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The **Encyclopedia** of **Cosmology**

Volume 1
Galaxy Formation and Evolution

Rennan Barkana

Giovanni G Fazio *editor*



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Galaxy Formation and Evolution

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The **Encyclopedia** of **Cosmology**

Volume 1
Galaxy Formation and Evolution

Rennan Barkana
Tel Aviv University

Editor
Giovanni G Fazio
Harvard Smithsonian Center for Astrophysics, USA

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Winston Churchill said:

“My most brilliant achievement was to persuade my wife to marry me”.

This volume is dedicated to my family — Riki, Or, Ariel, and my parents, who have been my companions on my career journey. It is also dedicated to Richard Feynman, whose writings first ignited my interest in physics. Feynman knew how to eloquently express the beauty of science¹:

“Poets say science takes away from the beauty of the stars — mere globs of gas atoms. I too can see the stars on a desert night, and feel them. But do I see less or more? The vastness of the heavens stretches my imagination — stuck on this carousel my little eye can catch one-million-year-old light. A vast pattern — of which I am a part... What is the pattern, or the meaning, or the why? It does not do harm to the mystery to know a little about it. For far more marvelous is the truth than any artists of the past imagined it. Why do the poets of the present not speak of it? What men are poets who can speak of Jupiter if he were a man, but if he is an immense spinning sphere of methane and ammonia must be silent?”

Feynman also wrote about the excitement of science²:

“We are very lucky to live in an age in which we are still making discoveries. It is like the discovery of America — you only discover it once”.

When he wrote this in 1965, Feynman was referring to the then golden age of particle physics. I believe that today we are living in a golden age of cosmology, particularly on the topics in Part II of this volume. May the reader experience the joy of discovery!

¹R. Feynman, *The Character of Physical Law* (1965). Modern Library. ISBN 0-679-60127-9.

²M. Sands, R. Feynman, R. B. Leighton, *The Feynman Lectures on Physics* (1964). AddisonWesley.

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Preface

This volume lays out the subjects of galaxy formation and evolution based on the current paradigm in cosmology. Part I presents the theoretical understanding and modeling of galaxy formation, including a brief treatment of galactic structure. While not intended to be completely comprehensive, it is meant to cover background knowledge that is important for graduate students and researchers working in cosmology or galaxy formation, and is written mostly in textbook style. It assumes pre-knowledge of cosmology (which is only briefly reviewed), and thus can be used as a source of advanced topics in a cosmology course, or as the basis for a follow-up course in advanced cosmology. The approach is astrophysical, focusing on galaxy formation and making only limited use of general relativity where necessary. When working through some of the more complicated sections, the reader may find encouragement in two famous quotes by Einstein: “Things should be made as simple as possible, but not any simpler”; and, “In the middle of every difficulty lies opportunity.” Part II builds on Part I by presenting the exciting subject of high-redshift galaxy formation, including topics such as cosmic dawn, the first stars, cosmic reionization, and 21-cm cosmology. Combining a review of progress on these topics with some detailed physics, it is meant to bring active researchers up to speed on recent work on galaxy formation at early times.

R. Barkana

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Part I

Basic Theory of Galaxy Formation

This part begins with a brief review of basic cosmology and of relevant topics in statistics, and then develops in detail the theory of galaxy formation as understood in modern cosmology; this includes linear perturbation theory, spherical collapse, and baryonic effects. After deriving some essential elements of stellar dynamics and of galactic structure, this part ends with a brief presentation of gravitational lensing.

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Chapter 1

Introduction

The theoretical basis of modern cosmology was laid out soon after Einstein's 1915 discovery of general relativity. Friedmann first worked out models of the expanding Universe, with Lemaitre adding the concepts of redshift and the initial Big Bang. Hubble's 1929 discovery of cosmic expansion was the first observational milestone. The hot Big Bang theory accumulated more substance as the first theoretical predictions of the cosmic microwave background (CMB) and of Big-Bang nucleosynthesis were made by Alpher, Gamow, and Herman in the 1940's. A watershed moment in observational cosmology came with the 1965 discovery of the CMB [1], which was the first direct evidence for the hot and dense initial state of the Universe. Meanwhile, astronomical evidence accumulated for the evolution of the Universe over time, as increasingly distant galaxies were discovered. Soon after quasars were identified as high-redshift objects, Gunn & Peterson [2] used their spectra (in 1965) to show that the inter-galactic gas around them was highly ionized; this was the first sign that the gas had undergone cosmic reionization, likely by the stars in early galaxies.

For a long time, the most fundamental questions about our Universe remained unanswered, including the energy contents of the Universe and the fate of its expansion. Observational evidence for dark matter emerged as early as 1933, from Zwicky's analysis of the Coma cluster of galaxies. This was not, however, taken seriously until the 1970's, when galactic rotation curves were shown by Vera Rubin to indicate the presence of massive amounts of unseen matter. Meanwhile, comparison of the observed abundances of the lightest elements with the predictions of Big Bang nucleosynthesis increasingly indicated a low cosmic baryon density, thus requiring the dark matter to be mostly non-baryonic. An early period of cosmic inflation was proposed by Guth in 1981 [3], helping to explain large-scale features of the Universe and the initial conditions needed for galaxy formation. Those initial conditions were finally discovered observationally in 1992, in the form of temperature anisotropy in the cosmic microwave background [4]; NASA's COBE satellite also confirmed the near-perfect black-body spectrum of the CMB [5], as expected in the hot Big Bang

model. A major surprise¹ was the 1998 discovery, using Type Ia supernovae as distance indicators, of accelerated expansion consistent with a large cosmological constant dominating the present energy density [6, 7]. Meanwhile, increasingly precise measurements were made of the CMB over a wide range of angular scales. The peak of the spectrum of temperature fluctuations at an angular scale of one degree was detected in 2000 by experiments including BOOMERanG [8] and MAXIMA [9]; these experiments also showed hints of higher-order acoustic peaks, which were unambiguously confirmed in 2003 by NASA’s WMAP satellite [10]. The fact that hundreds of individual points of the CMB angular fluctuation spectrum match the precise shape predicted by a model with 6 parameters (in the simplest Λ CDM model, i.e. cosmological constant Λ plus cold dark matter) is a scientific triumph that solidifies the entire theoretical framework of modern cosmology. Meanwhile, large galaxy redshift surveys detected the corresponding features in the power spectrum of the galaxy distribution [11, 12], including the fluctuation peak as well as baryon acoustic oscillations (the after-effects of baryons being carried along with the photons in sound waves in the early Universe). CMB polarization measurements have further confirmed the standard cosmological model, and have also detected the signature of cosmic reionization, although the originally high value of the optical depth [10] has been revised substantially, and the recent value from ESA’s Planck satellite is much lower [13].

Thus, the scientific study of the history of the Universe has undergone a tremendous acceleration in recent decades. Today it is expanding in many new directions. A major effort is directed towards increasingly large surveys of galaxies, one goal of which is to determine whether the cosmic equation of state is consistent with a cosmological constant. Other work focuses on further measurements of the CMB, including its polarization and spectral distortions. In between these two regimes, of the early Universe on the one hand and the recent one on the other, is the story of the formation of the first stars and quasars and their cosmic effects. This largely unmapped chapter in cosmic history is the subject of Part II of this volume.

Part I is meant to be a largely self-contained introduction to galaxy formation. To make it self-contained, it includes reviews of basic cosmology and of relevant statistical methods, and a brief derivation of the collisionless Boltzmann equation and its moments. The emphasis is on a physical understanding of galaxy formation, so linear perturbation theory, spherical collapse, and related topics are covered in detail. Extensive presentations of theoretical cosmology and galaxy formation can be found in many books, e.g. [14–19]. These books are good sources for subjects that are only briefly touched on here, such as particle cosmology (including cosmology of the very early Universe), perturbation theory in general relativity (including tensor

¹The author recalls attending a major cosmology conference as a student in the early 1990’s, where a vote was taken on the most likely cosmological model. Theorists voted for a flat matter-only Universe, observers for an open, low-density, matter-only Universe; almost no-one was in favor of a Universe dominated by a cosmological constant.

perturbations and the issue of gauge), and CMB physics (including the calculation and analysis of the anisotropies). Some of the material here, in particular in Chap. 4, was influenced by (my Ph.D. adviser) Ed Bertschinger's Les Houches lecture notes [20]. Chapters 6–8 present a selection of other topics that, I submit, any cosmologist should know. Anyone who studies galaxy formation should know something about the internal properties of galaxies, including our basic understanding of spiral structure. More generally, stellar dynamics is an important basis for understanding galaxies, galaxy clusters, and dark matter halos. The material in Chaps. 5 and 6 was mostly influenced by the standard advanced textbook of Binney & Tremaine [21]. Finally, gravitational lensing is both a physically and mathematically beautiful subject, and an important method with many astrophysical and cosmological applications.

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Chapter 2

Review of Cosmology

This volume assumes pre-requisite knowledge of basic cosmology and of standard methods of mathematical physics. This chapter presents just a brief review of essential elements of the expansion history of the Universe (more exhaustive expositions are available in standard textbooks such as those cited in the previous chapter).

2.1. The Friedmann–Robertson–Walker (FRW) metric

2.1.1. *The metric*

In general relativity, the metric for a space which is spatially homogeneous and isotropic is the Friedmann–Robertson–Walker (hereafter FRW) metric, which can be written in the form

$$ds^2 = dt^2 - a^2(t) \left[\frac{dr^2}{1 - k r^2} + r^2 d\Omega^2 \right], \quad (2.1)$$

where (r, θ, ϕ) are spherical comoving coordinates, t is the proper/physical time, $a(t)$ is the cosmic scale factor that describes expansion in time, and the angular area element is

$$d\Omega^2 = d\theta^2 + \sin^2 \theta d\phi^2. \quad (2.2)$$

Here $a(t)$ is dimensionless, r is called a “comoving” position coordinate since the scale factor has been factored out, and k has units of an inverse squared length. Unless otherwise indicated, we use units in which the speed of light $c \equiv 1$ (sometimes we still include factors of c in equations when this adds clarity). The constant k determines the geometry of the metric; it is positive in a closed Universe, zero in a flat Universe, and negative in an open Universe. While the closed Universe has a finite volume, the flat or open ones are infinite.¹

¹This is a good opportunity to mention Einstein’s clever quote: “Only two things are infinite, the Universe and human stupidity, and I’m not sure about the former.”

We can obtain an alternative form of the metric by factoring $a(t)$ out of the time variable as well, yielding the comoving or “conformal” time variable τ . If we also transform to a new radial variable χ in order to simplify the radial element, the metric becomes

$$ds^2 = a^2(\tau) [d\tau^2 - (d\chi^2 + \sin_k^2 \chi d\Omega^2)], \quad (2.3)$$

where

$$\sin_k \chi = \begin{cases} k^{-1/2} \sin(k^{1/2} \chi) & \text{if } k > 0 \text{ (closed)} \\ \chi & \text{if } k = 0 \text{ (flat)} \\ (-k)^{-1/2} \sinh[(-k)^{1/2} \chi] & \text{if } k < 0 \text{ (open)}. \end{cases} \quad (2.4)$$

These cases correspond to a closed, flat, or open spacetime geometry, as indicated. Here (χ, θ, ϕ) are another set of spherical comoving coordinates. In the important case of a spatially flat ($k = 0$) Universe, $r = \chi$ and the spatial parts of the two just-presented forms of the metric become identical. We follow the convention of setting the scale factor to unity today, i.e. $a(t_0) = a(\tau_0) = 1$.

2.1.2. Using the FRW metric

The FRW metric can be used to understand various properties of the space-time and the dynamics of its residents. In particular, stationary (“comoving”) observers at rest at a fixed (r, θ, ϕ) remain at rest,² with their physical separation increasing with time in proportion to $a(t)$. This case yields the relation between t and τ :

$$dr = d\chi = d\Omega = 0 \implies ds = dt = a d\tau. \quad (2.5)$$

If we consider a radial displacement at a fixed time, we obtain the physical (or “proper”) distance in the radial direction:

$$dt = d\Omega = d\tau = 0 \implies \Delta s = a(t) \int \frac{dr}{\sqrt{1 - kr^2}} = a(\tau) \Delta \chi. \quad (2.6)$$

The tangential (azimuthal) direction describe the physical area in the angular direction (e.g. on a spherical shell):

$$dt = d\tau = dr = d\chi = 0 \implies \text{Area} = 4\pi a^2 r^2 = 4\pi a^2 \sin_k^2 \chi. \quad (2.7)$$

An equivalent statement is that the angular diameter distance is

$$D_A = ar = a \sin_k \chi, \quad (2.8)$$

where a small angle θ corresponds to a transverse physical distance $D_A \theta$.

²This must formally be demonstrated by solving the geodesic equation, e.g. [1].

Another important special case is that of light, described by $ds = 0$. If, for simplicity, we consider a radial light ray, then

$$ds = d\Omega = 0 \implies \Delta t = a \int \frac{dr}{\sqrt{1 - kr^2}} = \text{physical distance}, \quad (2.9)$$

and also

$$\Delta\tau = \Delta\chi = \text{comoving distance}. \quad (2.10)$$

The comoving horizon (also the “particle horizon”) is the largest comoving distance from which light (or other causal influences) could have reached an observer at time t since the Big Bang (at which t and τ were zero):

$$\text{Comoving horizon} = \int_{t'=0}^t \frac{dt'}{a(t')} = \Delta\chi = \tau. \quad (2.11)$$

2.2. Cosmic expansion: dynamics

2.2.1. Hubble’s law

The “Hubble constant” (constant in space but varying in time) is defined as

$$H(t) \equiv \frac{d \ln a(t)}{dt} = \frac{1}{a} \frac{da}{dt} = \frac{\dot{a}}{a}, \quad (2.12)$$

where in general $\dot{p}$ denotes the time derivative of a variable p . In terms of the scale factor and the Hubble constant, the time variables are then

$$t = \int dt = \int \frac{da}{a H(a)}; \quad \tau = \int \frac{da}{a^2 H(a)}. \quad (2.13)$$

We will often use $\vec{x}$ for vector comoving positions (corresponding to the comoving spherical coordinates (χ, θ, ϕ) above), and $\vec{r}$ for the corresponding physical positions (unrelated to the r coordinate in Equation 2.1, which we will avoid using). Consider now two comoving observers, one at the origin and another at a fixed comoving position $\vec{x}$. The comoving displacement between them is $\vec{x}$, while the proper/physical displacement is $\vec{r} = a(t)\vec{x}$. The physical velocity is thus

$$\vec{v} = \frac{d\vec{r}}{dt} = \frac{da}{dt} \vec{x} = H a \vec{x} = H \vec{r}. \quad (2.14)$$

This is Hubble’s law.

2.2.2. Redshift of light

The cosmological redshift of light looks locally just like the classical Doppler shift corresponding to the recession velocity according to Hubble’s law. Imagine a photon emitted at the origin of the coordinates, and observed by a comoving observer

at $\vec{x}$. Then the velocity of the observer relative to the emitter is $v = x(da/dt)$ (where $x = |\vec{x}|$) as in Eq. (2.14), and the relation between the emitted and observed wavelength of the photon is $\lambda_{\text{obs}} = \lambda_{\text{emit}}(1 + v)$. Here we have used the Newtonian Doppler shift, assuming a small distance x (small compared to the horizon cH^{-1}) and thus $v \ll c$. The redshift z is defined through

$$1 + z \equiv \frac{\lambda_{\text{obs}}}{\lambda_{\text{emit}}} \implies z = v. \quad (2.15)$$

We can relate this to the cosmic expansion. The photon travels for a time $\Delta t = a\Delta\tau = ax$, so by the time it reaches the observer, the scale factor has increased to

$$\tilde{a} = a + \frac{da}{dt}\Delta t = a + \frac{da}{dt}ax = a \left(1 + \frac{da}{dt}x\right) = a(1 + v) = a(1 + z).$$

Finally, for an observer at $\tilde{a} = 1$, we obtain

$$\frac{\lambda(\tilde{a} = 1)}{\lambda(a)} = 1 + z = \frac{1}{a}. \quad (2.16)$$

This result ($\lambda \propto a$) is sometimes expressed intuitively as imagining that the wavelength of each photon simply expands along with the Universe. Note that we can subdivide a cosmological distance into many small segments, each of which can be analyzed as we have done here, together yielding $\lambda \propto a$ also over cosmologically large distances.³

2.2.3. Luminosity distance

Imagine a light emitter of luminosity L at a seen by a present observer at $a_0 = 1$. The luminosity distance D_L is defined so that the observed flux is

$$F \equiv \frac{L}{4\pi D_L^2}. \quad (2.17)$$

Using the metric of Eq. (2.3), we center the coordinates on the emitter and place the observer at a comoving radial distance χ . Then the emitted light spreads out over a sphere of physical area $4\pi a_0^2 \sin_k^2 \chi$. With $a_0 = 1$, we obtain

$$F = \frac{L}{4\pi \sin_k^2 \chi} a^2, \quad (2.18)$$

where we have added two factors of a due to the redshifting of energy and of the photon rate (which are both lower due to the cosmological redshift). The energy of

³Strictly speaking, in order to complete this argument, the statement must first be shown to be true locally including corrections from special relativity.

each photon is

$$h\nu \propto \frac{1}{\lambda}, \quad (2.19)$$

where ν is the physical frequency, so that the photon energy changes by a factor of a from emission to observation (see the previous subsection). For the interval between two photons, note that the interval $d\tau_{\text{O}}$ at the observer equals the interval $d\tau_{\text{E}}$ at the emitter, since each photon travels the same $\Delta\tau = \chi$ [Eq. (2.10)]. Thus, the relation between the physical time intervals is

$$dt_{\text{O}} = d\tau_{\text{O}} = d\tau_{\text{E}} = \frac{dt_{\text{E}}}{a},$$

i.e. the photon rate at the observer is multiplied by a factor of a . If we denote the comoving distance by D_{C} , we can summarize the various distances as:

$$D_{\text{A}} = a \sin_k \chi ; \quad D_{\text{C}} = \chi ; \quad D_{\text{L}} = \frac{1}{a} \sin_k \chi. \quad (2.20)$$

2.3. Cosmic expansion: kinematics

2.3.1. Friedmann equation

The Einstein field equations of general relativity, $G_{\mu\nu} = 8\pi G T_{\mu\nu}$, yield the Friedmann equation

$$H^2(t) = \frac{8\pi G}{3} \rho - \frac{k}{a^2}, \quad (2.21)$$

which relates the expansion of the Universe (through H) to its matter-energy content (through the energy density ρ) and curvature (through k). For an intuitive interpretation of this equation, consider an expanding Newtonian shell enclosing a fixed mass M with a radius increasing $\propto a$. Then Newtonian conservation of energy for the shell yields precisely the Friedmann equation [see Sec. 5.1], where H^2 comes from the kinetic energy term, ρ from the gravitational potential energy (which is negative so becomes positive on the right-hand side), and $-k$ is proportional to the conserved total energy of the shell (i.e. a negative total energy corresponds to a positive k , which is the case of an expansion that only reaches a finite radius and then re-collapses).

The field equations also yield a second independent equation:

$$d(\rho a^3) = -p d(a^3), \quad (2.22)$$

which is analogous to $dE = -p dV$ in classical thermodynamics (where E is the energy of a gas of pressure p in a volume V). This equation can be combined with the Friedmann equation to yield the acceleration of the expansion:

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3p). \quad (2.23)$$

Cosmic densities are often expressed relative to the critical density ρ_c , which is the density corresponding to a flat Universe. From Eq. (2.21),

$$\rho_c(t) \equiv \frac{3H^2(t)}{8\pi G}, \quad \Omega(t) \equiv \frac{\rho}{\rho_c}. \quad (2.24)$$

This definition yields an alternate form of the Friedmann equation:

$$\frac{k}{a^2} = H^2(t) [\Omega(t) - 1], \quad k = H_0^2 [\Omega_0 - 1], \quad (2.25)$$

where the expression on the right is the same equation at the present. This equation displays the relation between k (which sets the geometry of the Universe in the metric of Eq. (2.1) or Eq. (2.3)) and the contents of the Universe. It is an example of the deep geometry–density connection in general relativity.

2.3.2. Distribution functions and pressure

The subject of the distribution functions of particles will be dealt with extensively below. Here we only present a few basic results that are needed for describing the evolution of various components of the energy density of the Universe.

Define the distribution function $f(\vec{x}, \vec{q})$ for a collection of particles (such as a gas, a fluid, or particles in an N-body simulation) so that the number of particles in a phase-space volume $d^3x d^3q$ at position $\vec{x}$ and momentum $\vec{q}$ is

$$dN = f(\vec{x}, \vec{q}) d^3x d^3q. \quad (2.26)$$

Then the number density is

$$n(\vec{x}) = \int f(\vec{x}, \vec{q}) d^3q \quad (2.27)$$

and the total number of particles is $N = \int n d^3x$. The energy density (where as before $c = 1$) is

$$\rho = \int E(q) f(\vec{x}, \vec{q}) d^3q, \quad (2.28)$$

where $E(q) = \sqrt{(qc)^2 + (mc^2)^2}$ is the energy of a particle of momentum q .

Now consider the case of isotropic pressure. To calculate the pressure, consider the force dF in the z direction exerted by the particles on a piston (or the side of a box containing the particles) of small area dA that is perpendicular to the z direction (note: in this subsection z denotes a Cartesian coordinate, not redshift). The pressure is defined as

$$p = \frac{dF}{dA} = \frac{dq_z/dt}{dA},$$

where dq_z is the z component of momentum imparted to the piston, and we used the z component of Newton's law in the form that is also valid in special relativity.

Particles with z momentum q_z contribute $2q_z$ per particle to dq_z (with the factor of 2 due to elastic recoil). Particles with z velocity v_z can reach the piston during the time dt from as far away as $dz = v_z dt$. Thus,

$$dq_z = \int 2q_z \times f d^3q \times dA v_z dt.$$

Now, in general (in special relativity) $\vec{q} = \gamma m \vec{v}$, where m is the particle mass and $\gamma = 1/\sqrt{1-v^2}$. Also, isotropy implies:

$$\langle v_x^2 \rangle = \langle v_y^2 \rangle = \langle v_z^2 \rangle = \frac{1}{3} \langle v^2 \rangle,$$

where the averaging here is over all the particles at a given position. Thus, $\langle q_z v_z \rangle = \frac{1}{3} \langle q v \rangle$, but we must then add a factor of $1/2$ since in this averaging we must count only the half of particles headed towards the piston (and not in the opposite z direction). Thus,

$$dq_z = \frac{1}{3} \int q v f d^3q dA dt,$$

so that

$$p = \frac{1}{3} \int q v f d^3q. \quad (2.29)$$

Since $E = \gamma mc^2$, another way to write this result is

$$p = \int \frac{q^2 c^2}{3E(q)} f d^3q. \quad (2.30)$$

In the case of non-relativistic particles of mass m :

$$\text{Non-relativistic: } E = mc^2, \quad q = mv, \quad p \sim \rho \frac{\langle v^2 \rangle}{c^2}, \quad (2.31)$$

so that p is usually negligible when it competes with ρ (as in the cosmic expansion). For radiation:

$$\text{Photons: } v = c, \quad E = qc, \quad p = \frac{1}{3} \rho. \quad (2.32)$$

2.3.3. Equation of state

The equation of state is the relation between the pressure and density for each component of the cosmic energy density. Many components are described by the simple equation of state

$$p = w\rho, \quad (2.33)$$

where w is constant. Eq. (2.22) applies separately to each such component (when different components do not interact and exchange energy), which yields a simple

first-order differential equation whose solution is a power law in a :

$$\rho \propto a^{-n}, \text{ where } n = 3(1 + w). \quad (2.34)$$

If the cosmic density is dominated by such a single component, then the Friedmann equation (assuming $k = 0$ for simplicity) becomes

$$\dot{a} \propto a^{-\frac{1}{2}(1+3w)},$$

with solution

$$a(t) \propto \begin{cases} t^{\frac{2}{3(1+w)}} = t^{2/n} & \text{if } w > -1, \\ e^{\lambda t} & \text{if } w = -1. \end{cases} \quad (2.35)$$

In terms of conformal time,

$$a(\tau) \propto \tau^{\frac{2}{1+3w}} \propto \tau^{\frac{2}{n-2}}, \quad (2.36)$$

if $w > -1/3$.

One special case is a matter-dominated Universe, where the energy density is due to non-relativistic matter. In this case the pressure is negligible, so that $w = 0$, $\rho \propto a^{-3}$ (corresponding to volume dilution of a fixed number of particles), and the expansion is $a \propto t^{2/3} \propto \tau^2$.

Another important case is a radiation-dominated Universe, where photons (or any ultra-relativistic particles) dominate. In this case $w = 1/3$ [Eq. (2.32)], $\rho \propto a^{-4}$ [corresponding to volume dilution plus redshifting $\propto 1/a$ of the energy per photon: Eq. (2.19)], and the expansion is $a \propto t^{1/2} \propto \tau$.

A third important case is that of vacuum energy (or cosmological constant), which has a constant density ($n = 0$) and thus $w = -1$. Intuitively, in order for an expanding volume to maintain a constant energy density, the total energy in the volume must increase, which requires effectively a negative pressure (i.e. $p dV$ work with the opposite sign of that of a classical gas). In this case, a is exponential in t (corresponding to the rapid expansion during cosmic inflation), and τ converges as $a \rightarrow \infty$ (if the expansion is started at a finite a in order to avoid the divergence at $a \rightarrow 0$). This convergence corresponds to the horizons established during inflation, as the rapid expansion cuts off different regions from future causal contact with each other. In the present Universe, which is dominated by a cosmological constant, our cosmic Local Group region is also expected to be gradually cut off from communication with the rest of the Universe [2].

While not usually physically significant, we can also list the case of no acceleration $w = -1/3$ [Eq. (2.23)], which corresponds to $\rho \propto a^{-2}$ (effectively like the curvature term in the next equation, below), $a \propto t$, and an exponential dependence on τ .

We can now derive the standard picture of the expansion history of the Universe given its contents. If we let Ω_m , Ω_Λ , and Ω_r denote the present contributions to Ω

from matter, vacuum energy, and radiation, respectively, the Friedmann equation [Sec. 2.3.1] becomes

$$H^2(t) = H_0^2 \left[\frac{\Omega_m}{a^3} + \Omega_\Lambda + \frac{\Omega_r}{a^4} + \frac{\Omega_k}{a^2} \right], \quad (2.37)$$

where H_0 and $\Omega_0 = \Omega_m + \Omega_\Lambda + \Omega_r$ are the present values of H and Ω , respectively, and we define

$$\Omega_k \equiv -\frac{k}{H_0^2} = 1 - \Omega_0. \quad (2.38)$$

Matter here includes cold dark matter as well as a contribution Ω_b from baryons.

Currently, the best-fit cosmological parameters of this Λ CDM model, based on the full data of the Planck satellite [3], are: $h = 0.678$, where the present Hubble constant is defined as

$$H_0 = 100 h \text{ km s}^{-1} \text{ Mpc}^{-1}, \quad (2.39)$$

and a flat Universe ($\Omega_k = 0$)⁴ with matter density parameter $\Omega_m = 0.308$ and the rest (adding up to unity) in a cosmological constant (i.e. $\Omega_\Lambda = 0.692$). Also, $\Omega_b = 0.0484$, so that baryons make up 15.7% of the total matter density, and dark matter the other 84.3%. In the standard hot Big Bang model, the Universe is initially hot and the energy density is dominated by radiation. This is followed by matter domination, while Λ is dominant today and into the future. The critical density of Eq. (2.24) has the present value

$$\rho_c = 8.63 \times 10^{-30} \left(\frac{h}{0.678} \right)^2 \text{ g cm}^{-3}. \quad (2.40)$$

It is also useful to note that

$$H_0^{-1} = 9.784 h^{-1} \text{ Gyr}; \quad cH_0^{-1} = 2.998 h^{-1} \text{ Gpc}. \quad (2.41)$$

We note that cosmologists often explicitly take out the Hubble constant in expressions, e.g. distances in cosmology are expressed in units of h^{-1} Mpc (and wavenumbers in h Mpc⁻¹). This is to some degree a remnant of an earlier time when h was uncertain by nearly a factor of two. Now that h has been determined to equal ≈ 0.7 to good accuracy, it may be preferable to simply use units of Mpc, and specify the assumed h in case it is needed for precise comparisons.

⁴If Ω_k is allowed to vary, then its measured value is consistent with zero, with a 95% one-sided uncertainty of 0.004 if all observational constraints are combined.

2.3.4. Einstein–de Sitter (EdS) limit

In the particularly simple Einstein–de Sitter (EdS) model ($\Omega_m = 1$, $\Omega_\Lambda = \Omega_r = \Omega_k = 0$), the scale factor varies as $a(t) \propto t^{2/3}$. Even models with non-zero Ω_Λ or Ω_k approach the Einstein–de Sitter behavior at high redshifts, i.e. when

$$(1+z) \gg \max \left[\Omega_k/\Omega_m, (\Omega_\Lambda/\Omega_m)^{1/3} \right], \quad (2.42)$$

as long as we do not reach extremely early times at which Ω_r cannot be neglected. The approach to EdS is particularly rapid in practice given that current observations imply $\Omega_k \approx 0$.

In this EdS regime (which we will also refer to as the high- z regime), $H(t) \approx 2/(3t)$. Also in this regime,

$$H(z) \approx H_0 \frac{\sqrt{\Omega_m}}{a^{3/2}}, \quad (2.43)$$

and the age of the Universe is

$$t \approx \frac{2}{3H_0\sqrt{\Omega_m}} (1+z)^{-3/2} = 5.49 \times 10^8 \left(\frac{\Omega_m h^2}{0.141} \right)^{-1/2} \left(\frac{1+z}{10} \right)^{-3/2} \text{ yr}. \quad (2.44)$$

The comoving (or particle) horizon of Eq. (2.11) is, in the high-redshift EdS limit (and not including an early period of inflation):

$$\eta \approx 5.05 \left(\frac{\Omega_m h^2}{0.141} \right)^{-1/2} \left(\frac{1+z}{10} \right)^{-1/2} \text{ Gpc}. \quad (2.45)$$

Also note that the comoving cosmic mean density of matter in the Universe is:

$$\bar{\rho}_m = 2.65 \times 10^{-30} \left(\frac{\Omega_m h^2}{0.141} \right) \frac{\text{g}}{\text{cm}^3} = 3.91 \times 10^{10} \left(\frac{\Omega_m h^2}{0.141} \right) \frac{M_\odot}{\text{Mpc}^3}, \quad (2.46)$$

where the second expression uses particularly convenient units for galaxy formation. The physical density at redshift z is higher than the comoving one by a factor of $(1+z)^3$.

2.4. Redshifting of peculiar velocity

The real Universe is inhomogeneous, and observers are not purely comoving. If an observer's physical position is $\vec{r}$ in physical coordinates and $\vec{x}$ in comoving coordinates, i.e. $\vec{r} = a(t)\vec{x}$, then the velocity is

$$\frac{d\vec{r}}{dt} = H\vec{r} + a\frac{d\vec{x}}{dt}. \quad (2.47)$$

The first term is the recession velocity corresponding to Hubble expansion, and the second term is called the *peculiar velocity*, i.e. the velocity that remains when measured relative to a nearby comoving observer.

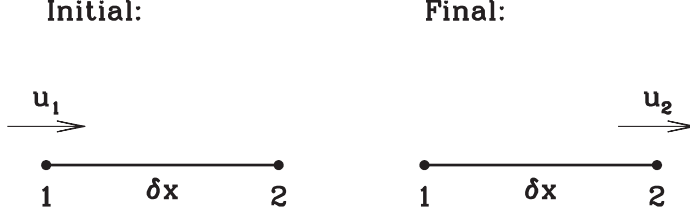


Fig. 2.1. Sketch for calculating the redshifting of peculiar velocity.

To calculate the redshifting of peculiar velocity, consider two comoving observers, #1 and #2, situated at a fixed comoving separation δx in the x direction (see Fig. 2.1). Now imagine a rocket that starts at the position of observer #1 at the initial time, with a velocity u_1 (that is possibly relativistic) in the $+x$ direction, i.e. towards observer #2. Suppose the rocket reaches the position of observer #2 after a physical time δt . The peculiar velocity of the rocket at observer #1 is u_1 , and we wish to determine its peculiar velocity u_2 at observer #2.

We use the frame of reference of observer #1. The velocity δv of observer #2 in this frame (relative to #1) is the Hubble velocity $H\delta r$, where $\delta r = a\delta x$. Note that in some expressions we assume that H and a do not change significantly over the small, cosmologically insignificant time interval δt ; more precisely, we calculate everything to lowest order in the small parameter δv — which is in units of c . Now, the time interval is given by $u_1\delta t = \delta r$. Thus,

$$\delta v = \frac{1}{a} \frac{da}{dt} u_1 \delta t = \frac{u_1}{a} \delta a,$$

where δa is the change in a during the time δt .

When the rocket reaches #2, its velocity is still u_1 with respect to #1 (changes in this velocity are second order in δv). To find the velocity of the rocket with respect to observer #2 at that time, we use relativistic velocity subtraction (since we are allowing u_1 to be relativistic):

$$u_2 = \frac{u_1 - \delta v}{1 - u_1 \delta v} \simeq (u_1 - \delta v)(1 + u_1 \delta v) \simeq u_1 - (1 - u_1^2) \delta v.$$

Thus, the change in the peculiar velocity is

$$\delta u = - (1 - u_1^2) \delta v = - (1 - u_1^2) \frac{u_1}{a} \delta a.$$

Now consider the peculiar momentum q of the rocket/particle (assumed of mass m) and how it changes:

$$q = \frac{mu_1}{\sqrt{1 - u_1^2}}, \quad \delta q = \frac{m\delta u}{(1 - u_1^2)^{3/2}},$$

where we used the relativistic expression for momentum and then took its derivative with respect to velocity. The above expression for δu can be written as:

$$a \delta u (1 - u_1^2)^{3/2} + \delta a u_1 (1 - u_1^2)^{-1/2} = 0.$$

Multiplied by m , this becomes $a \delta q + q \delta a = 0$. This is the same as $\delta(qa) = 0$, which finally yields:

$$q \propto \frac{1}{a}. \quad (2.48)$$

This is a general result for the redshifting of the peculiar momentum, valid for velocities of order the speed of light as well as for non-relativistic motion; in the latter case it is equivalent to the simple $u \propto 1/a$ in terms of the peculiar velocity u . For a photon, we have seen that its energy redshifts as $1/a$ [Eq. (2.19)], so its momentum is $q = E \propto 1/a$, in agreement with Eq. (2.48). As in the case of the redshifting of light [Sec. 2.2.2], more generally we can subdivide a cosmological distance into many small segments, each of which can be analyzed as we have done here, together yielding $q \propto 1/a$ also over cosmologically large distances.

We note that the redshifting of momentum, i.e. its decline with time, foreshadows an important result that we will encounter later, namely that cosmic expansion suppresses perturbations. The decrease of peculiar velocities tends to erase non-uniformity, bringing moving objects closer to the pure Hubble expansion that characterizes a homogeneous Universe.

2.5. Temperature evolution of gas and radiation

Consider photons in the Universe, observed today as the cosmic microwave background (CMB). They follow a thermal distribution early on, due to frequent scatterings and interactions in the dense and hot, early Universe. Eventually, though, the interactions die out, and each photon travels freely in the expanding Universe. Assume that the photons are in a Planck distribution of temperature T_1 at some scale factor a_1 , i.e. the number of photons per unit volume in the frequency range $\omega_1 \rightarrow \omega_1 + d\omega_1$ is:

$$n_1(\omega_1) d\omega_1 = \frac{1}{\pi^2 c^3} \frac{\omega_1^2 d\omega_1}{e^{\hbar\omega_1/kT_1} - 1}. \quad (2.49)$$

Note that here we are using the angular frequency $\omega = 2\pi\nu$. Then at a later time, at scale factor a_2 , we denote the number per volume $n_2(\omega_2) d\omega_2$. Now, in free expansion, the number per volume goes down as $(a_1/a_2)^3$, and as we have seen [Eq. (2.48)], the frequency redshifts so that $\omega_2 = \omega_1 a_1/a_2$ and thus also $d\omega_2 = d\omega_1 a_1/a_2$. Therefore,

$$n_2(\omega_2) d\omega_2 = \left(\frac{a_1}{a_2}\right)^3 \frac{1}{\pi^2 c^3} \frac{\omega_1^2 d\omega_1}{e^{\hbar\omega_1/kT_1} - 1} = \frac{1}{\pi^2 c^3} \frac{\omega_2^2 d\omega_2}{e^{\hbar\omega_2/kT_2} - 1},$$

where

$$T_2 = T_1 \frac{a_1}{a_2}. \quad (2.50)$$

This calculation implies that the photons maintain a Planck distribution, but with a redshifting effective temperature, $T \propto 1/a$. This is consistent with the redshifting of photon energy given that the typical photon energy is $\propto k_B T$, where k_B is the Boltzmann constant.

We note that we have only shown here that the Planck distribution is maintained once the photons are decoupled. However, there is an intermediate regime during which interactions (in which energy is exchanged and/or photons are created) gradually freeze out. In this regime, in fact, the Planck distribution is not perfectly maintained. The resulting CMB spectral distortions, plus distortions resulting from energy injections (either those expected in standard cosmology or from more speculative possibilities), are a target for future telescopes, and represent an active field of research [4–6].

Moving from photons to a non-relativistic gas, in the latter case the temperature T_b (where the subscript indicates baryons) measures the kinetic energy of random velocities (which are peculiar). Thus, the redshifting of peculiar velocity (see the previous sub-section) yields

$$k_B T_b \propto \langle v^2 \rangle \propto \frac{1}{a^2}, \quad (2.51)$$

where we assumed a decoupled non-interacting gas (i.e. one that is not heated or cooled by interactions with the CMB, atomic radiative processes, etc.). Thus, under adiabatic cosmic expansion, non-relativistic gas cools faster than the CMB.

We can now understand the cosmic evolution of radiation. The cosmic energy density of radiation is given by the Stefan–Boltzmann law as

$$\rho_r = \frac{\pi^2}{30} \frac{k_B^4}{(\hbar c)^3} g_* T^4, \quad (2.52)$$

where T is the temperature of the Planck spectrum of the photons, and the effective number of degrees of freedom for the energy density, including relativistic species, is (except for very early times)

$$g_* = 2 + \frac{7}{8} \times 2 \times 3.046 \times \left(\frac{4}{11} \right)^{4/3} = 3.384. \quad (2.53)$$

Here the effective number of degrees of freedom is 2 for photons; for neutrinos there is an extra factor of $7/8$ since they are fermions, 3.046 is the effective number of neutrino species (including a small correction caused by a non-thermal spectral distortion during electron-positron annihilation [7]), and the $(4/11)^{4/3}$ factor is due to the increase in temperature of the photons relative to the neutrinos by a factor of $(11/4)^{1/3}$ during electron-positron annihilation. The temperature today is 2.725 K

for the CMB photons (and thus 1.95 K for the neutrinos), giving a present radiation density

$$\rho_r = 7.80 \times 10^{-34} \text{ g cm}^{-3}. \quad (2.54)$$

Comparing to the critical density [Eq. (2.40)] yields

$$\Omega_r = 9.04 \times 10^{-5} \left(\frac{h}{0.678} \right)^{-2}. \quad (2.55)$$

Also, the number density of photons is

$$n_\gamma = \frac{\zeta(3)}{\pi^2} \frac{k_B^3}{(\hbar c)^3} 2T^3 = 408 \text{ cm}^{-3}, \quad (2.56)$$

where ζ is the Riemann zeta function.

The transition from radiation domination to matter domination occurred at the redshift of matter-radiation equality z_{eq} , where $\Omega_r (1 + z_{\text{eq}}) = \Omega_m$, so that

$$1 + z_{\text{eq}} = 3390 \frac{\Omega_m h^2}{0.141}. \quad (2.57)$$

After equality the Universe remained hot enough that the gas was ionized, and electron-photon scattering effectively coupled the baryonic matter and the radiation. At $z \sim 1100$ the temperature dropped below ~ 3000 K and the protons and electrons recombined to form neutral hydrogen (“cosmic recombination”). The photons then decoupled and traveled freely until the present, when they are observed as the CMB. However, Compton scattering with the residual electron fraction (of a few $\times 10^{-4}$) kept the gas temperature coupled to the CMB temperature until $z \sim 200$ (“thermal decoupling”). A small fraction ($\sim 6\%$) of the photons re-scattered at low redshift, on the free electrons generated after cosmic reionization (by UV radiation from early stars). More recently, the cosmological constant began to dominate over the matter density at

$$1 + z_\Lambda = \left(\frac{\Omega_\Lambda}{\Omega_m} \right)^{1/3}, \quad (2.58)$$

which gives $z_\Lambda = 0.310$ with currently measured cosmological parameters.

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Chapter 3

Statistics of Galaxy Formation

Since theoretical models of galaxy formation generally make their predictions statistically, in this chapter we briefly introduce a number of important subjects in statistics. These include random fields, correlation functions, and power spectra.

3.1. Random fields and correlation functions

3.1.1. *Continuous and discrete fields*

A random field in space (at a given time) is a spatial distribution of random variables, i.e. a field that has a particular value at each point in space, with the values depending on a stochastic process. Statistical calculations in galaxy formation involve both continuous and discrete random fields. A prime example of a continuous field is the density ρ . We often use the alternate variable

$$\delta(\vec{x}) \equiv \frac{\rho(\vec{x}) - \bar{\rho}}{\bar{\rho}} = \frac{\rho(\vec{x})}{\bar{\rho}} - 1, \quad (3.1)$$

where the average density

$$\bar{\rho} \equiv \langle \rho(\vec{x}) \rangle, \quad (3.2)$$

so that $\langle \delta(\vec{x}) \rangle = 0$. Each average in these expressions denotes a statistical average, i.e. an average (at a fixed position $\vec{x}$) over an ensemble of random fields with particular statistical properties. We normally assume the *Ergodic Hypothesis*: An average over all positions $\vec{x}$ (or, in practice, over a sufficiently large volume) is equal to an ensemble average at a fixed $\vec{x}$.

A discrete field is a random field that describes discrete (rather than continuous) entities. A closely related concept is a point process, which is a random process whose realizations consist of sets of discrete points. A standard example of a discrete

field in cosmology is the Poisson model of galaxies, whereby the actual number of galaxies in a given volume is a realization of a Poisson distribution whose mean value is given by a continuous random field. Specifically, in a small volume d^3x , the probability of having a galaxy is

$$dP = n(\vec{x}) d^3x, \quad (3.3)$$

where $n(\vec{x})$ is the galaxy number density (a continuous field). We can write it as:

$$n(\vec{x}) = \bar{n}[1 + \delta_n(\vec{x})], \quad (3.4)$$

in analogy with Eq. (3.1) for $\rho(\vec{x})$.

3.1.2. The correlation function

The two-point correlation function (sometimes simply called “the correlation function”) is defined as the following ensemble average, given two points in space $\vec{x}_1$ and $\vec{x}_2$:

$$\xi(r_{12}) = \langle \delta(\vec{x}_1) \delta(\vec{x}_2) \rangle, \quad (3.5)$$

where $r_{12} = |\vec{x}_1 - \vec{x}_2|$ is the distance between the two points. Here we have made the usual assumption in cosmology of a statistically homogeneous and isotropic random field, so that ξ depends only on the distance between the two selected points ($\vec{x}_1$ and $\vec{x}_2$) and not on anything else (such as the direction between them or their absolute location).

The correlation function expresses a property of the joint distribution of the random field ρ at two points. Specifically:

$$\langle \rho(\vec{x}_1) \rho(\vec{x}_2) \rangle = \langle \bar{\rho}[1 + \delta(\vec{x}_1)] \bar{\rho}[1 + \delta(\vec{x}_2)] \rangle = \bar{\rho}^2 [1 + \xi(r_{12})]. \quad (3.6)$$

In the discrete example of the Poisson model of galaxies, the joint probability of having galaxies in a small volume d^3x_1 near $\vec{x}_1$ and in a small volume d^3x_2 near $\vec{x}_2$ (also called the pair distribution function) is

$$dP(\vec{x}_1, \vec{x}_2) = n(\vec{x}_1) n(\vec{x}_2) d^3x_1 d^3x_2 = \bar{n}^2 d^3x_1 d^3x_2 [1 + \delta_n(\vec{x}_1)][1 + \delta_n(\vec{x}_2)]. \quad (3.7)$$

The ensemble average (also called the expectation or expected value) of this is

$$\langle dP(\vec{x}_1, \vec{x}_2) \rangle = \bar{n}^2 d^3x_1 d^3x_2 [1 + \langle \delta_n(\vec{x}_1) \delta_n(\vec{x}_2) \rangle^d]. \quad (3.8)$$

Here we have added a subscript “d” for discrete, which symbolizes the fact that in the discrete case, shot noise is added to the continuous correlation function, as shown in the next subsection.

3.1.3. Shot noise and the discrete correlation function

With the Poisson model of galaxies, consider a given volume V . Then the expected number of galaxies in this volume is

$$\bar{N} = \langle N \rangle = \left\langle \int dV n(\vec{x}) \right\rangle = \int dV \langle n(\vec{x}) \rangle = \bar{n}V. \quad (3.9)$$

To find $\langle N^2 \rangle$, we divide V into a large number of very small cells of volume V_i (centered on position x_i), where the index i runs over all the cells. Thus,

$$V = \sum_i V_i, \quad (3.10)$$

and the number of galaxies in cell i (assumed to be at most one due to the smallness of the volume V_i) is

$$N_i = \begin{cases} 1 & \text{with probability } n(\vec{x}_i)V_i \\ 0 & \text{with probability } 1 - n(\vec{x}_i)V_i. \end{cases} \quad (3.11)$$

Thus,

$$\langle N_i \rangle = \langle 1 \cdot [n(\vec{x}_i)V_i] + 0 \cdot [1 - n(\vec{x}_i)V_i] \rangle = \langle n(\vec{x}_i)V_i \rangle = \bar{n}V_i. \quad (3.12)$$

This calculation illustrates that we have here two levels of random processes: $n(\vec{x})$ is a random field (and the $\langle \rangle$ brackets denote its expectation value), and on top of this we also have the Poisson process which yields an integer number of galaxies.

We now calculate pair expectation values, including the Poisson process. Similarly to Eq. (3.12), we find

$$\langle N_i^2 \rangle = \langle 1^2 \cdot [n(\vec{x}_i)V_i] + 0^2 \cdot [1 - n(\vec{x}_i)V_i] \rangle = \bar{n}V_i. \quad (3.13)$$

A bit more complicated is the result for an unequal pair ($i \neq j$). Only the term where neither cell has zero galaxies contributes here:

$$\begin{aligned} \langle N_i N_j \rangle &= \langle 1^2 \cdot [n(\vec{x}_i)V_i] [n(\vec{x}_j)V_j] \rangle = \langle n(\vec{x}_i)n(\vec{x}_j) \rangle V_i V_j \\ &= \bar{n}^2 V_i V_j [1 + \langle \delta_n(\vec{x}_1)\delta_n(\vec{x}_2) \rangle] = \bar{n}^2 V_i V_j [1 + \xi(r_{ij})]. \end{aligned} \quad (3.14)$$

Here we have explicitly separated out the Poisson process, leaving the expectation value of a product of continuous $n(\vec{x})$ fields, resulting in the continuous correlation function ξ appearing in the last step.

We now sum up the individual cells in order to compute

$$\begin{aligned}\langle N^2 \rangle &= \left\langle \sum_i N_i \sum_j N_j \right\rangle = \sum_i \langle N_i^2 \rangle + \sum_{i \neq j} \langle N_i N_j \rangle \\ &= \sum_i \bar{n} V_i + \bar{n}^2 \int \int dV_1 dV_2 [1 + \xi(r_{12})] = \bar{N} + \bar{N}^2 + \bar{n}^2 \int \int dV_1 dV_2 \xi(r_{12}).\end{aligned}\quad (3.15)$$

Note that in the transition to the integrals, we took advantage of the fact that adding $i = j$ to the double integral makes an infinitesimal (and thus negligible) difference (assuming that $\int d^3 r \xi(r)$ converges at $r \rightarrow 0$). The result for the variance is thus

$$\sigma_N^2 = \langle (N - \bar{N})^2 \rangle = \langle N^2 \rangle - \bar{N}^2 = \bar{N} + \bar{n}^2 \int \int dV_1 dV_2 \xi(r_{12}). \quad (3.16)$$

The $\bar{N}$ term in the variance is the shot noise. On its own, it would give a relative uncertainty $\sigma_N/\bar{N} = 1/\sqrt{\bar{N}}$, the well-known result for Poisson noise.

Another way to express this final result, without having to explicitly calculate the Poisson process as we have done, is to define an effective discrete correlation function:

$$\langle \delta_n(\vec{x}_1) \delta_n(\vec{x}_2) \rangle^d \equiv \xi(r_{12}) + \bar{n}^{-1} \delta_D(\vec{x}_1 - \vec{x}_2), \quad (3.17)$$

in terms of a Dirac δ function. To see that this works, first note that in the continuous case, we would simply get

$$\langle N^2 \rangle = \int \int dV_1 dV_2 \langle n(\vec{x}_1) n(\vec{x}_2) \rangle = \bar{n}^2 \int \int dV_1 dV_2 [1 + \xi(r_{12})]. \quad (3.18)$$

If we plug Eq. (3.17) into the double integral in this expression, the added term gives

$$\bar{n}^2 \int \int dV_1 dV_2 [\bar{n}^{-1} \delta_D(\vec{x}_1 - \vec{x}_2)] = \bar{n} \int dV_1 = \bar{N}, \quad (3.19)$$

which is precisely the shot-noise term.

3.1.4. Higher-order correlation functions

In cosmology, much of the focus is on pair correlation functions. Here we briefly introduce higher-order correlation functions (e.g. [3]), with the three-point and four-point correlation functions as specific examples. We consider the continuous case, for simplicity.

For the three-point correlation function we apply Eq. (3.6) to the case of three positions:

$$\rho(\vec{x}_1)\rho(\vec{x}_2)\rho(\vec{x}_3) = \bar{\rho}^3[1 + \delta(\vec{x}_1)][1 + \delta(\vec{x}_2)][1 + \delta(\vec{x}_3)]. \quad (3.20)$$

The expectation value is

$$\langle \rho(\vec{x}_1)\rho(\vec{x}_2)\rho(\vec{x}_3) \rangle = \bar{\rho}^3[1 + \xi_{12} + \xi_{23} + \xi_{31} + \xi_{123}]. \quad (3.21)$$

Here, e.g. $\xi_{12} \equiv \langle \delta(\vec{x}_1)\delta(\vec{x}_2) \rangle$, and $\xi_{123} \equiv \langle \delta(\vec{x}_1)\delta(\vec{x}_2)\delta(\vec{x}_3) \rangle$. The corresponding expression for the four-point correlation function is

$$\begin{aligned} \langle \rho(\vec{x}_1)\rho(\vec{x}_2)\rho(\vec{x}_3)\rho(\vec{x}_4) \rangle = \\ \bar{\rho}^4[1 + \xi_{12} + \xi_{23} + \xi_{31} + \xi_{14} + \xi_{24} + \xi_{34} + \xi_{123} + \xi_{124} + \xi_{134} + \xi_{234} + \xi_{1234}]. \end{aligned} \quad (3.22)$$

Next, we briefly introduce the concept of a cluster expansion in terms of cumulants (also called irreducible moments), which here will be denoted with a subscript *c*. For each expectation value of a product of δ 's, the cumulants are defined as that part that cannot be expressed in terms of lower-order expectation values. In the one-point case, simply

$$\langle \delta \rangle = \langle \delta \rangle_c. \quad (3.23)$$

This expectation value equals zero for δ as defined above, but the cluster expansion is a more general result valid also for random fields that do not average to zero. The two-point case is

$$\xi_{12} = \langle \delta_1 \delta_2 \rangle = \langle \delta_1 \rangle_c \langle \delta_2 \rangle_c + \langle \delta_1 \delta_2 \rangle_c. \quad (3.24)$$

Here we wrote, e.g. δ_1 as shorthand for $\delta(\vec{x}_1)$. The cumulant $\langle \delta_1 \delta_2 \rangle_c$ is the non-trivial contribution to $\langle \delta_1 \delta_2 \rangle$ that does not arise as a result of lower-order cumulants (one-point, in this case). In the case where $\langle \delta \rangle = 0$, we see that $\xi_{12} = \langle \delta_1 \delta_2 \rangle_c$. The three-point case is more interesting:

$$\begin{aligned} \xi_{123} = \langle \delta_1 \delta_2 \delta_3 \rangle = \langle \delta_1 \rangle_c \langle \delta_2 \rangle_c \langle \delta_3 \rangle_c + \langle \delta_1 \delta_2 \rangle_c \langle \delta_3 \rangle_c + \langle \delta_2 \delta_3 \rangle_c \langle \delta_1 \rangle_c \\ + \langle \delta_3 \delta_1 \rangle_c \langle \delta_2 \rangle_c + \langle \delta_1 \delta_2 \delta_3 \rangle_c. \end{aligned} \quad (3.25)$$

In the case of $\langle \delta \rangle = 0$, we again see that $\xi_{123} = \langle \delta_1 \delta_2 \delta_3 \rangle_c$, although this is not true for higher-order cases. For a Gaussian random field, $\langle \delta_1 \delta_2 \delta_3 \rangle_c = 0$, and the same is true for all higher-order cumulants. In other words, a Gaussian random field only has a non-zero two-point (and possibly one-point) cumulant, hence the correlation function completely determines all higher-order expectation values in this very special case. As a final example, we consider the four-point expectation value, and go straight to the case of $\langle \delta \rangle = 0$, for which

$$\xi_{1234} = \langle \delta_1 \delta_2 \delta_3 \delta_4 \rangle = \langle \delta_1 \delta_2 \rangle_c \langle \delta_3 \delta_4 \rangle_c + \langle \delta_1 \delta_3 \rangle_c \langle \delta_2 \delta_4 \rangle_c + \langle \delta_1 \delta_4 \rangle_c \langle \delta_2 \delta_3 \rangle_c + \langle \delta_1 \delta_2 \delta_3 \delta_4 \rangle_c. \quad (3.26)$$

For a Gaussian random field, the final term vanishes, and we get simply

$$\xi_{1234} = \xi_{12}\xi_{34} + \xi_{13}\xi_{24} + \xi_{14}\xi_{23}. \quad (3.27)$$

3.1.5. *Random walks and mean free paths*

We include here a brief reminder of the basic properties of a random walk. Suppose a total displacement (“walk”) $\Delta\vec{x}$ starting at the origin is composed of many individual steps:

$$\Delta\vec{x} = \sum_{i=1}^n \Delta\vec{x}_i.$$

Suppose each step traverses a distance that is Gaussian distributed, with root-mean-square σ_i , in a random (i.e. uniformly distributed) direction. Then $\langle\Delta\vec{x}_i\rangle = \vec{0}$ and $\langle|\Delta\vec{x}_i|^2\rangle = \sigma_i^2$. Thus,

$$\langle\Delta\vec{x}\rangle = \sum_{i=1}^n \langle\Delta\vec{x}_i\rangle = \vec{0}, \quad (3.28)$$

while, assuming that the individual steps are statistically independent of each other,

$$\langle|\Delta\vec{x}|^2\rangle = \sum_{i=1}^n \langle|\Delta\vec{x}_i|^2\rangle = \sum_{i=1}^n \sigma_i^2. \quad (3.29)$$

In the simple case of statistically equal steps, where $\sigma_i = \sigma$ for every i , this gives the famous $\sqrt{N}$ increase of the root-mean-square distance:

$$\sqrt{\langle|\Delta\vec{x}|^2\rangle} = \sqrt{N}\sigma. \quad (3.30)$$

A particular example of a random walk is one in which each step corresponds to a particle traveling between collisions, with potential collision partners which we will call the target particles. The chance that a particle has a collision in a distance dx is $n\sigma_c dx$, where n is the number of target particles per unit volume and σ_c is the effective cross-sectional area for collision. Let P be the probability that the particle has not yet had a collision after distance x . Then the probability $P + dP$ at $x + dx$ equals the probability P (of no collision up to x) times the probability $1 - n\sigma_c dx$ (of also no collision between x and $x + dx$), i.e. $dP = -Pn\sigma_c dx$. Since $P(0) = 1$,

$$P(x) = e^{-n\sigma_c x}. \quad (3.31)$$

Then the mean free path, the average distance traveled between collisions, is

$$l \equiv \langle x \rangle = \int_0^\infty x |dP| = (n\sigma_c)^{-1}. \quad (3.32)$$

Note that if the travel direction is random after each collision, then the vector $\langle \vec{x} \rangle = 0$. The variance is

$$\langle x^2 \rangle = \int_0^\infty x^2 |dP| = 2l^2. \quad (3.33)$$

Here the random walk is made up of segments from one collision to the next, and the total root-mean-square distance after N segments is, given Eq. (3.30),

$$\sqrt{\langle |\Delta \vec{x}|^2 \rangle} = \sqrt{2N} l. \quad (3.34)$$

3.2. The power spectrum

The power spectrum is the Fourier-space analogue of the pair correlation function. It plays a prominent role in both theoretical and observational cosmology.

3.2.1. Definition

To begin, we describe the spatial form of the density fluctuations in Fourier space, in terms of (three-dimensional) Fourier components $\hat{\delta}(\vec{k})$, where the Fourier transform and its inverse are:

$$\hat{\delta}(\vec{k}) = \int d^3x \delta(\vec{x}) e^{-i\vec{k} \cdot \vec{x}}; \quad \delta(\vec{x}) = \int \frac{d^3k}{(2\pi)^3} \hat{\delta}(\vec{k}) e^{i\vec{k} \cdot \vec{x}}. \quad (3.35)$$

We note that the $(2\pi)^3$ factor is sometimes switched (or split) between these two equations, and this choice also affects the numerical coefficients in other equations in this section; thus, care must be taken when comparing results that use different conventions for this factor within the definitions of the Fourier transform and its inverse. Here we have introduced the comoving wavevector $\vec{k}$, whose magnitude k is the comoving wavenumber which is equal to 2π divided by the wavelength. Note that, from the definition, $\hat{\delta}(-\vec{k}) = \hat{\delta}^*(\vec{k})$ if $\delta(\vec{x})$ is real.

The variance of the various $\vec{k}$ -modes is described in terms of the power spectrum (or power spectral density) $P(k)$. The rough idea is $P(k) \sim \langle |\hat{\delta}(\vec{k})|^2 \rangle$, but the precise mathematical definition is:

$$\langle \hat{\delta}(\vec{k}) \hat{\delta}^*(\vec{k}') \rangle = (2\pi)^3 P(k) \delta_D(\vec{k} - \vec{k}'), \quad (3.36)$$

where δ_D is the (three-dimensional) Dirac delta function. A useful representation of the Dirac delta function is

$$\delta_D(\vec{k}) = \int d^3x e^{\pm i\vec{k} \cdot \vec{x}}. \quad (3.37)$$

Note that $P(k)$ (which here is the power spectrum of δ) has units of volume; more generally, the power spectrum of some quantity has units of volume times the square of the units of that quantity.

3.2.2. Relation to the correlation function

The Fourier relation between the power spectrum and the correlation function is known as the Wiener–Khinchine theorem:

$$P(k) = \int d^3x e^{-i\vec{k}\cdot\vec{x}} \xi(r); \quad \xi(r) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{x}} P(k), \quad (3.38)$$

where $r = |\vec{x}|$.

As an example, we derive $\xi(r)$ from $P(k)$:

$$\begin{aligned} \xi(r) &= \langle \delta(\vec{x}_1) \delta(\vec{x}_2) \rangle = \left\langle \int \frac{d^3k_1}{(2\pi)^3} \hat{\delta}(\vec{k}_1) e^{i\vec{k}_1\cdot\vec{x}_1} \int \frac{d^3k_2}{(2\pi)^3} \hat{\delta}(\vec{k}_2) e^{i\vec{k}_2\cdot\vec{x}_2} \right\rangle \\ &= \left\langle \int \frac{d^3k_1}{(2\pi)^3} \frac{d^3k_2}{(2\pi)^3} e^{i(\vec{k}_1\cdot\vec{x}_1 + \vec{k}_2\cdot\vec{x}_2)} (2\pi)^3 P(k_1) \delta_D(\vec{k}_1 + \vec{k}_2) \right\rangle \\ &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{x}_1 - \vec{x}_2)} P(k), \end{aligned} \quad (3.39)$$

where $r = |\vec{x}_1 - \vec{x}_2|$, and we called the remaining integration variable $\vec{k}$ instead of $\vec{k}_1$. This verifies Eq. (3.38), but we can now continue and get a simpler expression. We let $\vec{x} \equiv \vec{x}_1 - \vec{x}_2$, and use spherical coordinates (k, θ, ϕ) for $\vec{k}$, defined relative to $\vec{x}$ as the z -direction. Thus, θ is the angle between $\vec{x}$ and $\vec{k}$, and $\vec{k} \cdot \vec{x} = kr \cos \theta$. The 3-D integral is

$$\int d^3k = \int_0^\infty k^2 dk \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi.$$

The ϕ integral is trivial. To do the θ integral, we let $\mu = \cos \theta$, so that $\int_0^\pi \sin \theta d\theta = \int_{-1}^1 d\mu$. The θ integral in $\xi(r)$ is

$$\int_{-1}^1 d\mu e^{ikr\mu} = \frac{e^{ikr\mu}}{ikr} \Big|_{-1}^1 = \frac{2 \sin(kr)}{kr}.$$

Thus, we obtain

$$\xi(r) = \frac{1}{2\pi^2} \int_0^\infty k^2 dk P(k) \frac{\sin(kr)}{kr}. \quad (3.40)$$

A few notes: $\sin(x)/x$ is also $j_0(x)$, the spherical Bessel function (of the first kind) of order 0. It is also sometimes called the sinc function (where the value at $x = 0$ is usually defined to equal unity, which is the $x \rightarrow 0$ limit of this expression). The special case $\xi(0) = \langle \delta(\vec{x}) \delta(\vec{x}) \rangle$ is simply the variance σ^2 of δ (although when $r \rightarrow 0$ in Eq. (3.40), the integral can diverge at $k \rightarrow \infty$, as is the case for the standard cold dark matter power spectrum where $P(k) \propto k^{-3}$ at large k). This $r \rightarrow 0$ limit

shows that the contribution of modes near a given wavenumber k to the variance of δ is

$$\frac{d\sigma^2(k)}{d \ln k} = \frac{k^3 P(k)}{2\pi^2}, \quad (3.41)$$

where $\sigma^2(k)$ is the integral of Eq. (3.40) with an upper integration limit of k (and a dummy integration variable of, say, $\tilde{k}$ instead of k).

Intuitively, when $kr \ll 1$ then the two points at distance r are on the same part of the wave of wavenumber k , so the full correlation is counted as for $r = 0$. When kr is not small, the points are on different parts of the wave, there is sometimes destructive interference, and the sinc function effectively averages over the various directions of the waves. We also note that the inverse relation to Eq. (3.40) is similarly derived to be

$$P(k) = \int d^3x e^{-i\vec{k} \cdot \vec{x}} \xi(r) = 4\pi \int_0^\infty r^2 dr \xi(r) \frac{\sin(kr)}{kr}. \quad (3.42)$$

3.2.3. The discrete power spectrum

Thus far in this section we have considered the continuous Fourier transform and power spectrum. In the discrete case, we consider a finite cube of length L and volume $V = L^3$. The cube effectively represents infinite space if we assume periodic boundary conditions (as is usually the case in numerical simulations in cosmology).

We set up a grid in both x and k -space. The spacings are $\Delta x = L/N$ (where each side L is divided into N intervals) and $\Delta k = 2\pi/L$, and the grid points on which the discrete fields are evaluated are:

$$\vec{x}_{\vec{j}} = (j_x, j_y, j_z) \Delta x, \quad 0 \leq j_x, j_y, j_z < N,$$

$$\vec{k}_{\vec{l}} = (l_x, l_y, l_z) \Delta k, \quad 0 \leq l_x, l_y, l_z < N,$$

where the j 's and l 's are integers. The discrete Fourier transform and its inverse are

$$\hat{\delta}(\vec{k}_{\vec{l}}) = \sum_{\vec{j}} e^{-i\vec{k}_{\vec{l}} \cdot \vec{x}_{\vec{j}}} \delta(\vec{x}_{\vec{j}}); \quad \delta(\vec{x}_{\vec{j}}) = N^{-3} \sum_{\vec{l}} e^{i\vec{k}_{\vec{l}} \cdot \vec{x}_{\vec{j}}} \hat{\delta}(\vec{k}_{\vec{l}}), \quad (3.43)$$

where here it is the N^{-3} factor that is sometimes switched or split between these two equations. The discrete version of the Dirac delta function is the Kronecker delta, which is useful for manipulating discrete Fourier transforms due to the relation:

$$\sum_{\vec{j}} e^{i\vec{k}_{\vec{l}} \cdot \vec{x}_{\vec{j}}} = N^3 \delta_{\vec{l}\vec{0}}^{\text{K}}, \quad (3.44)$$

where $\delta_{\vec{l}\vec{0}}^{\text{K}}$ is zero except that it equals unity if $\vec{l}$ equals the zero vector $\vec{0} = (0, 0, 0)$.

The discrete power spectrum is defined as

$$(\Delta k)^3 P(\vec{k}_l) = \left\langle \left| \hat{\delta}(\vec{k}_l) \right|^2 \right\rangle. \quad (3.45)$$

In analogy with Eq. (3.38), this also equals the Fourier transform of the correlation function, i.e.

$$(\Delta k)^3 P(\vec{k}_l) = \sum_{\vec{j}} e^{-i\vec{k}_l \cdot \vec{x}_{\vec{j}}} \text{Corr}(\vec{x}_{\vec{j}}), \quad (3.46)$$

where

$$\text{Corr}(\vec{x}_{\vec{j}}) = \sum_{\vec{m}} \delta(\vec{x}_{\vec{m}}) \delta(\vec{x}_{\vec{m}} + \vec{x}_{\vec{j}}), \quad (3.47)$$

where $\vec{m}$ denotes an integer vector with the same range as $\vec{j}$ or $\vec{l}$ above. Here $\vec{x}_{\vec{j}}$ plays the role of the difference vector of the two positions at which the δ 's are evaluated, and as before, δ is assumed to be real and periodic with respect to the box.

3.3. Detailed correlation function example

3.3.1. Cox process

Statistics such as the power spectrum and correlation function, while seemingly simple to define, are in fact rather subtle concepts. Indeed, it is not easy to give a specific example where they can be calculated directly from scratch. Here we present the Cox process as a complete, worked example of calculating a correlation function, with the motivation that seeing such a detailed derivation will help the reader develop some intuition as to what it is that the correlation function actually measures.

In the Cox process, one places segments of length L randomly, and then chooses random points on each segment. Specifically, let us assume a total volume V , with densities of n_S segments per volume, and λ_P points per unit length on each segment. Then the total number of segments is on average $\langle N_S \rangle = n_S V$, each on average with $\langle N_P \rangle = \lambda_P L$ points. The mean total number of points is $\langle N \rangle = n_S V \lambda_P L$. The volume density of points (or the probability of finding a point per unit volume) is $dP/dV = n_S \lambda_P L$. An example of a simulated Cox process is shown in Fig. 3.1.

3.3.2. Analytical calculation of $\xi(r)$

In general [Sec. 3.1.2], the probability of having points at positions $\vec{x}_1$ and $\vec{x}_2$ is

$$dP(\vec{x}_1, \vec{x}_2) = \bar{n}^2 dV_1 dV_2 [1 + \xi(r_{12})].$$

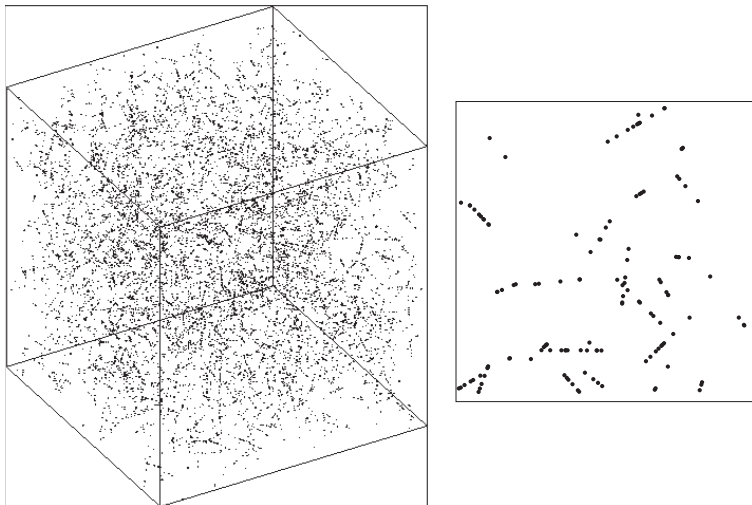


Fig. 3.1. An example of the Cox process, simulated on a cube of side-length 100, with parameters $n_S = 0.001$ and $L = 10$. The entire cube is shown (left panel) as well as a projected thin (depth 10) slice of size 40×40 (right panel). From [1].

We place $\vec{x}_1$ at the origin, and write r instead of r_{12} and dV instead of dV_2 . Then the conditional probability of the second point given the first one is

$$dP(r|0) = \bar{n}[1 + \xi(r)]dV. \quad (3.48)$$

For the Cox process, the correlation arises only from pairs on the same segment. Thus, $\xi(r) = 0$ for $r > L$. We now calculate the result for $r \leq L$.

We do this in two steps, where for the first step we assume $L \rightarrow \infty$ (or, more precisely, $L \gg r$). Then the probability of having point #2 on the same segment as #1 is

$$\left[\frac{dx dy}{4\pi r^2} \times 2 \right] \times [\lambda_P dz] = \frac{\lambda_P}{2\pi r^2} dV.$$

This is derived as follows (see the top panel of Fig. 3.2).

We are given point #1, so it is on a segment. Since $L \rightarrow \infty$, this segment is really an infinite straight line that passes through the origin. In the above expression, the first factor on the left-hand side is the chance that this infinite line passes through the volume element dV at point #2 (a distance r away). Since the angular direction of this line is uniformly distributed, this chance is the solid angle $dx dy$ subtended by the volume element $dV = dx dy dz$, divided by the total solid angle 4π (elsewhere in this volume z usually denotes redshift, but here it is the spatial coordinate in the direction from point #1 to #2). This is actually multiplied by two, since the infinite line goes in two directions (like a two-sided jet in astronomy). If the infinite line does indeed go in the correct direction, then the chance that there is a point

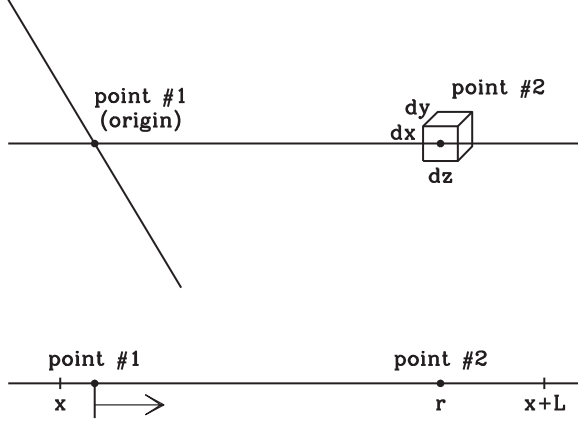


Fig. 3.2. Sketches to help calculate the correlation function of the Cox process (see text). Top panel: For step 1, this shows an infinite line (analogous to a two-sided jet) passing through the two points (plus another passing only through the first one), and a volume element $dV = dx dy dz$ around point #2. Bottom panel: For step 2, this shows positions x and $x + L$ (representing the two ends of a finite segment) measured from point #1 in the direction of point #2 (which is at position r). The example position shows a negative value of x .

at the correct distance (to within dz) is the linear density of points on the segment times dz ; this is the second factor on the left-hand side. The total probability of having a point at #2 (at a distance r from the origin 0) is the uncorrelated part (where point #2 is on some other segment; this is simply the overall volume density of points times dV) plus the correlated part (where point #2 is on the same segment as point #1):

$$dP(r|0) = n_S \lambda_P L dV + \frac{\lambda_P}{2\pi r^2} dV. \quad (3.49)$$

By definition, the correlated term equals the uncorrelated term times the correlation function. Thus, in this case,

$$\xi(r) = \frac{1}{2\pi r^2 n_S L}. \quad (3.50)$$

In the second step, we now add the fact that L is finite. To do this, we first imagine an infinite segment in the correct direction from point #1 to #2 (as in step one, where point #2 is at position $r > 0$), and then we randomly cut segments of length L out of it. We wish to find the probability that point #2 is on the same segment as point #1, given that point #1 is indeed on a segment. Thus, we imagine that we perform a random cut on the infinite segment, with the left-hand edge of the segment at a distance x from the origin (see the bottom panel of Fig. 3.2). We are only interested in a segment that contains point #1, which is at position 0. Since the segment is of length L , this means that $x < 0 < x + L$, which is equivalent to the condition $-L < x < 0$ on x . Since segments are distributed randomly, the random

variable x is uniformly distributed within this length L . Now, point #2 is also on the same segment if $x < r < x + L$, equivalent to $r - L < x < r$. For this condition to be satisfied together with the previous condition (from considering point #1), we must first of all have $r < L$ (otherwise, the two conditions on x do not overlap at all). If, indeed, $r < L$, then the two conditions combine to give $r - L < x < 0$. Thus, out of the possible range L , a segment of length $L - r$ corresponds to point #2 being on the same segment as point #1. The correlated part of the probability $dP(r|0)$ that point #2 is on the same segment as point #1 is equal to the probability that point #2 would be on the same segment if it were infinite (step 1 above), times the probability that it is close enough to also be on the same finite segment. The latter factor is $(L - r)/L$, which multiplies $\xi(r)$ from step 1. The final answer is therefore

$$\xi(r) = \begin{cases} \frac{1}{2\pi n_S} \left(\frac{1}{r^2 L} - \frac{1}{r L^2} \right) & \text{if } r < L \\ 0 & \text{if } r \geq L. \end{cases} \quad (3.51)$$

3.3.3. Numerical Cox process with extensions

The numerically-calculated correlation function for the simulated Cox process indeed matches (in both shape and normalization) the analytical result calculated in the previous subsection (Fig. 3.3). In the numerical simulation, it is easy to also extend the Cox process by adding random shifts to each point, in order to further develop a feel for what the correlation function measures (Fig. 3.3). If the shifts are generated according to a power-law distribution that falls with distance (so that most shifts are small), this suppresses the correlation function on small scales, and makes it less steeply falling with r . If, instead, the random shifts are Gaussian distributed, this completely erases the short-range correlations, causing $\xi(r)$ to become flat on scales roughly below the root-mean-square value of the shift.

3.4. Statistical topics in galaxy formation

In this section we briefly present several statistical topics that are particularly relevant to galaxy formation.

3.4.1. Gaussian random fields

We begin by briefly summarizing the properties of Gaussian random fields. These are important since perturbations in cosmology are often assumed to be given by a Gaussian random field, as is the case (to high accuracy) for fluctuations generated by cosmic inflation [2]. The statistical properties of such fields are determined by $P(k)$, or equivalently $\xi(r)$. In particular, all higher-order cumulants (higher than order two) vanish. Also, all sets of linear functions or functionals of $\delta(\vec{x})$ are multivariate normal variables. However, this is not the case for non-linear functions or functionals.

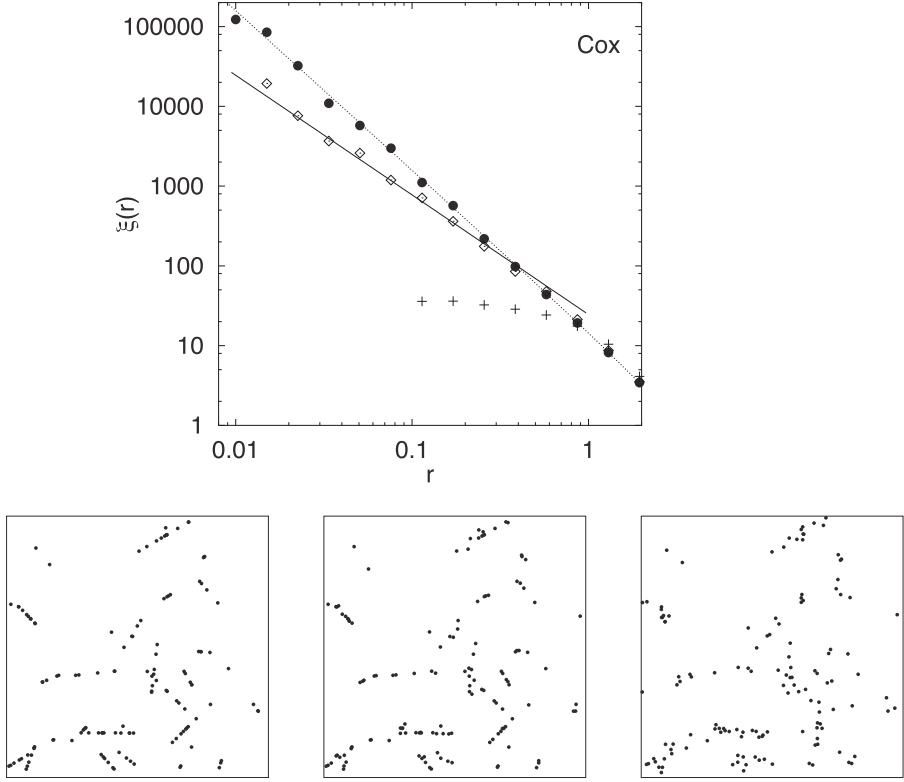


Fig. 3.3. Top panel: The numerically-calculated correlation function for the Cox process and simple extensions. The correlation function is shown for the numerically simulated Cox process (solid points; corresponding theoretical prediction shown as dotted curve) of Fig. 3.2, with added power-law shifts (open diamonds; power law for comparison shown as solid curve), and with added Gaussian shifts (+ signs). In the cases with added shifts, each point generated by the Cox process is then randomly shifted, by a distance that is generated according to a density probability function $\propto r^{-0.75}$ in the range $r = 0 - 1$ (in the power-law case), or according to a normal distribution with $\sigma = 0.5$ (in the Gaussian case). Bottom panel: A projected thin (depth 10) slice of size 40×40 of the box, for the Cox process (left), with added power-law shifts (middle), and with added Gaussian shifts (right). From [1].

For a Gaussian random field, different $\vec{k}$ -modes are statistically independent, each with a random phase. In the discrete case, $\text{Re } \hat{\delta}(\vec{k}_T)$ and $\text{Im } \hat{\delta}(\vec{k}_T)$ are, for each $\vec{k}_T$, Gaussian variables with zero mean and with variance equal to $P(\vec{k}_T)(\Delta k)^3/2$. Alternatively, we can use the magnitude and phase description,

$$\hat{\delta}(\vec{k}_T) = |\hat{\delta}(\vec{k}_T)| e^{i\phi(\vec{k}_T)}. \quad (3.52)$$

Then $0 \leq \phi(\vec{k}_T) < 2\pi$ is uniformly distributed (and the field is said to have “random phases”), and the magnitude $|\hat{\delta}(\vec{k}_T)|$ follows a Rayleigh distribution:

$$p(x) dx = \sigma^{-2} e^{-x^2/(2\sigma^2)} x dx, \quad \sigma^2 = P(\vec{k}_T)(\Delta k)^3, \quad x \geq 0. \quad (3.53)$$

3.4.2. Window functions

In models of galaxy formation, we are often interested in considering not the raw, un-smoothed, density field, but the smoothed density field:

$$\bar{\delta}(\vec{x}) = \int d^3x' W(|\vec{x}' - \vec{x}|) \delta(\vec{x}'). \quad (3.54)$$

This expression averages the value of δ over the region near $\vec{x}$, with the weighting of values at various distances r from $\vec{x}$ given by the window function $W(r)$. By definition, $\bar{\delta}(\vec{x})$ is a convolution of δ and W . Since a convolution in real space is equivalent to a simple multiplication in $\vec{k}$ (Fourier) space, we roughly expect

$$\hat{\hat{\delta}} \sim \tilde{W} \cdot \hat{\delta}, \quad \left\langle \left(\hat{\hat{\delta}} \right)^2 \right\rangle \sim \tilde{W}^2 P(k),$$

where $\tilde{W}$ is the Fourier transform of W . The correlation function $\bar{\xi}$ of the smoothed density field is then related to the power spectrum via Eq. (3.40), and the variance is the correlation function at zero spacing. The precise relation is

$$\bar{\xi}(r) = \frac{1}{2\pi^2} \int_0^\infty k^2 dk \tilde{W}^2(k) P(k) \frac{\sin(kr)}{kr}, \quad (3.55)$$

and then $\sigma^2 = \bar{\xi}(0)$, where we define

$$\tilde{W}(k) = \int d^3x W(r) e^{-i\vec{k} \cdot \vec{x}}. \quad (3.56)$$

Since W only depends on r , $\tilde{W}$ depends only on the magnitude k . Also note that

$$\tilde{W}(0) = \int d^3x W(r) = 1, \quad (3.57)$$

where the final equality is a standard normalization condition for the window function W .

There are a few particular window functions that are especially useful in galaxy formation. These include the top hat¹ (in real space):

$$W_{\text{TH}}(r) = \theta \left(1 - \frac{r}{R} \right) [4\pi R^3/3]^{-1}, \quad (3.58)$$

where the last factor ensures normalization, and we used the step function

$$\theta(x) \equiv \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0. \end{cases} \quad (3.59)$$

¹The name “top hat” refers to the hat-like shape of the window function in a one-dimensional plot, say versus x at $y = z = 0$.

This window function smooths δ (at each point) uniformly within a sphere of radius R . Equation (3.56) gives

$$\tilde{W}_{\text{TH}}(k) = \frac{3}{x^3} (\sin x - x \cos x) = \frac{3}{x} j_1(x), \quad (3.60)$$

where $x = kR$ and $j_1(x)$ is the spherical Bessel function of order 1. Note that the magnitude of $\tilde{W}_{\text{TH}}(k)$ decreases rapidly at $kR \gg 1$, because such k values correspond to short waves that produce fluctuations on scales below R , and these fluctuations average out when the field is smoothed on the scale R .

Another important example is the Gaussian window function, which is symmetric (i.e. has a similar form) between real space and Fourier space:

$$W_{\text{G}}(r) = e^{-r^2/(2R^2)} (2\pi R^2)^{-3/2}, \quad \tilde{W}_{\text{G}} = e^{-k^2 R^2/2}. \quad (3.61)$$

Finally, a top hat in $\vec{k}$ -space (also called a sharp Fourier space filter) is

$$\tilde{W}_{\text{K}}(k) = \theta(1 - kR_{\text{K}}), \quad (3.62)$$

where R_{K} is a parameter with units of length. This corresponds to

$$W_{\text{K}}(r) = \frac{1}{2\pi^2 R_{\text{K}}^3} \frac{1}{x} j_1(x), \quad (3.63)$$

where $x = r/R_{\text{K}}$ (Note that this window function has a normalization difficulty because of the lack of convergence of Eq. (3.57) in this case, at the $r \rightarrow \infty$ end).

The normalization of the (linear) power spectrum in cosmology can be specified at any one scale. It is common tradition to use the parameter σ_8 , which is the standard deviation σ of δ smoothed with a top hat window function W_{TH} for $R = 8 h^{-1}$ Mpc. This spatial scale corresponds roughly to the mass scale of galaxy clusters.

3.4.3. Model for biased galaxy formation

Galaxy formation is “biased”, which means that galaxies tend to cluster, i.e. form in fairly tight groups rather than being randomly distributed. Some intuition can be developed for biased galaxy formation by considering a Gaussian random field δ at two different positions [3]. Note that it is also possible to consider here the same field but smoothed with a window function, since the smoothed field is a Gaussian random field as well.

In this subsection we use the shorthand $\delta_1 = \delta(\vec{x}_1)$ and $\delta_2 = \delta(\vec{x}_2)$. We first note that

$$\langle \delta_1^2 \rangle = \langle \delta_2^2 \rangle = \xi(0), \quad \langle \delta_1 \delta_2 \rangle = \xi(r). \quad (3.64)$$

We now define

$$\delta_+ = \delta_1 + \delta_2, \quad \delta_- = \delta_1 - \delta_2. \quad (3.65)$$

Then

$$\langle \delta_+ \delta_- \rangle = \langle \delta_1^2 - \delta_2^2 \rangle = 0, \quad (3.66)$$

which means that δ_+ and δ_- are independent (Two jointly normal random variables that are uncorrelated are independent). Their variances are

$$\sigma_{\pm}^2 \equiv \langle \delta_{\pm}^2 \rangle = 2[\xi(0) \pm \xi(r)], \quad (3.67)$$

so the joint probability distribution (ignoring the normalization factors which are unimportant here) is

$$\begin{aligned} P(\delta_1, \delta_2) &\propto P(\delta_+, \delta_-) \propto \exp \left\{ -\frac{1}{2} \left[\frac{\delta_+^2}{\sigma_+^2} + \frac{\delta_-^2}{\sigma_-^2} \right] \right\} \\ &= \exp \left\{ -\frac{1}{2} \left[\frac{(\delta_1 + \delta_2)^2}{2[\xi(0) + \xi(r)]} + \frac{(\delta_1 - \delta_2)^2}{2[\xi(0) - \xi(r)]} \right] \right\}. \end{aligned} \quad (3.68)$$

Then the conditional probability is

$$\begin{aligned} P(\delta_2 | \delta_1) &= \frac{P(\delta_1, \delta_2)}{P(\delta_1)} \propto \frac{P(\delta_1, \delta_2)}{\exp\{-\delta_1^2/[2\xi(0)]\}} \\ &\propto \exp \left\{ -\frac{1}{2} \frac{\xi(0)}{\xi^2(0) - \xi^2(r)} \left[\delta_2 - \delta_1 \frac{\xi(r)}{\xi(0)} \right]^2 \right\}. \end{aligned} \quad (3.69)$$

This conditional probability is thus a normal variable, and its mean and variance can be read off the final expression.

We are particularly interested in the mean value:

$$\langle \delta_2 | \delta_1 \rangle = \delta_1 \frac{\xi(r)}{\xi(0)}. \quad (3.70)$$

To apply this to galaxy formation, we note that galaxies tend to form earlier and in larger numbers in regions with high density, due to the enhanced gravity there. Specifically, as we show later, the condition for forming a galactic halo can be seen as equivalent to having the density cross above a fixed threshold, and any overall enhancement in the density of a region makes it more likely that parts of it will pass above that threshold (see Sec. 5.4 and Sec. 11.2). We thus see that at a distance r from a large δ_1 (where galaxy formation is enhanced), the expected value of δ_2 is positive as well (compared to the unconditional mean of zero), which implies an enhanced number density of galaxies there as well. This bias is typically large nearby, and falls off with distance as $\xi(r)$ declines.

In galaxy formation we are often interested in galactic halos of a particular mass, which formed from the mass in a sphere of (comoving) radius R . In this case,

as noted above, the same result holds but with all quantities referring to the density field smoothed with a top hat (or other choice of window function).

3.4.4. Limber's equation

It is sometimes useful to consider the angular correlation function of galaxies. This might be the case with large samples of galaxies that do not have accurately measured distances (e.g. if spectroscopic redshifts are unavailable and photometric redshifts are not sufficiently accurate). The relation between the three-dimensional correlation function and the projected angular one is known as Limber's equation.

We follow here the basic setup of the discrete correlation function of Sec. 3.1.2 but neglect shot noise. Consider a small solid angle $d\Omega$. Then the number of galaxies within it is

$$dN = \int_0^\infty r^2 dr n(r) d\Omega. \quad (3.71)$$

When $dN \ll 1$, this is really the probability dP of finding a galaxy. Then the mean probability of finding a galaxy is

$$\langle dP \rangle = \bar{\nu} d\Omega, \quad (3.72)$$

where the mean angular density of galaxies is

$$\bar{\nu} = \int_0^\infty r^2 dr \bar{n}(r). \quad (3.73)$$

The joint probability of finding galaxies in two angular directions is

$$\langle dP_{12} \rangle = \bar{\nu}^2 d\Omega_1 d\Omega_2 [1 + w(\theta)], \quad (3.74)$$

where this equation defines the angular correlation function $w(\theta)$.

To evaluate it, we integrate radially within the cones corresponding to each of the two small solid angle elements:

$$dP_{12} = dN_1 dN_2 = \int \int r_1^2 dr_1 \bar{n}(r_1) [1 + \delta(r_1)] r_2^2 dr_2 \bar{n}(r_2) [1 + \delta(r_2)] d\Omega_1 d\Omega_2. \quad (3.75)$$

The expectation value is then

$$\langle dP_{12} \rangle = d\Omega_1 d\Omega_2 \int \int r_1^2 dr_1 r_2^2 dr_2 \bar{n}(r_1) \bar{n}(r_2) [1 + \xi(r_{12})], \quad (3.76)$$

where the separation between distance r_1 in the direction of $d\Omega_1$ and distance r_2 in the direction of $d\Omega_2$ is given by the law of cosines in terms of the angle θ separating

the two directions:

$$r_{12} = (r_1^2 + r_2^2 - 2r_1r_2 \cos \theta)^{1/2}. \quad (3.77)$$

Finally, we obtain

$$w(\theta) = \frac{1}{\bar{\nu}^2} \int \int (r_1 r_2)^2 dr_1 dr_2 \bar{n}(r_1) \bar{n}(r_2) \xi(r_{12}). \quad (3.78)$$

References

- [1] Martinez, V., Saar, E. In: *Astronomical Data Analysis II*. Edited by Jean-Luc Starck & Fionn D. Murtagh, Proceedings of the SPIE, 4847 (2002) 86.
- [2] E. W. Kolb, M. S. Turner, *The Early Universe*, Addison-Wesley, Redwood City, CA, 1990.
- [3] P. J. E. Peebles, *Principles of Physical Cosmology*, Princeton University Press, Princeton, 1993.

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Chapter 4

Linear Perturbation Theory and the Power Spectrum

4.1. Preview of perturbation theory

In this section we use the special case of spherical symmetry for a relatively simple derivation of perturbation theory. While this is a restricted case, it does preview some aspects of general perturbation theory, and helps develop physical intuition since the spherical derivation has a rather Newtonian flavor.

4.1.1. *Mass-radius relations for initial halo mass*

While halos do not form out of precisely spherical regions, this simplistic image does serve an important role in analyzing galaxy and halo formation. One reason is that the linear spherical collapse problem, studied in the next subsection, gives an accurate preview of the most important results of the full, non-spherical linear analysis that follows later in this chapter. Another is that non-linear spherical collapse plays a critical role in the successful Press–Schechter model of halo abundances, as shown in the next chapter. These successes provide more than sufficient justification for using the spherical picture for some rough estimates of various scaling relations. A simple example of such a relation is that between mass and radius.

Assuming a spherical region, a halo of mass M forms out of an initial (i.e. when $\delta \rightarrow 0$) region of comoving radius R , where

$$M = \frac{4}{3}\pi\bar{\rho}_0 R^3 = 1.64 \times 10^8 \left(\frac{\Omega_m h^2}{0.141} \right) \left(\frac{R}{100 \text{ kpc}} \right)^3 M_\odot. \quad (4.1)$$

The inverse relation is:

$$R = 84.8 \left(\frac{\Omega_m h^2}{0.141} \right)^{-1/3} \left(\frac{M}{10^8 M_\odot} \right)^{1/3} \text{ kpc}. \quad (4.2)$$

4.1.2. Linear spherical collapse

In a homogeneous expanding Universe, the acceleration equation is Eq. (2.23) in Chap. 2. If we now consider a comoving observer at a fixed comoving position $\vec{x}$ (measured from some origin of the coordinates), its physical position is simply $\vec{R} = a\vec{x}$. Thus, it satisfies the equation

$$\ddot{\vec{R}} = \ddot{a}\vec{x} = -\frac{4}{3}\pi G(\rho + 3p)\vec{R}. \quad (4.3)$$

We now assume spherical symmetry (about the origin), and follow a shell enclosing a fixed mass of matter, M . The symmetry assumption greatly simplifies things due to *Birkhoff's Theorem* in general relativity (GR), which states that the evolution in spherical symmetry depends only on the enclosed energy components. Thus, if the shell has a different density than the mean Universe enclosing it, then the shell effectively contains a perturbed Universe of its own, while outside it the Universe is at its mean density. In order to apply Eq. (4.3), we assume that the density and pressure are uniform inside the shell (so that the Friedmann equation applies to the perturbed Universe). We separate out the matter (here including both dark matter and gas, assuming that the effect of gas pressure is negligible) from other components (radiation and a cosmological constant, for example). Then for the mean Universe, the acceleration equation in Eq. (2.23) can be written as

$$\frac{\ddot{a}}{a} = -\frac{4}{3}\pi G\bar{\rho}_m - \frac{4}{3}\pi G(\rho + 3p)_{\text{rest}}, \quad (4.4)$$

where subscript “m” denotes matter while “rest” is everything else. While the mean Universe contains the mean matter density $\bar{\rho}_m$, the portion enclosed within our shell may contain a different density $\rho_m = M/[4\pi R^3/3]$ (note that M is the fixed enclosed mass of matter, not including other energy components). Equation (4.3) can then be written in the form

$$\ddot{R} = -\frac{GM}{R^2} - \frac{4}{3}\pi G(\rho + 3p)_{\text{rest}}R. \quad (4.5)$$

Here we have essentially managed to apply the special case of a comoving observer to the motion of *any* observer, but only within a particular, strong assumption of symmetry.

We wish to express the evolution in terms of the overdensity δ of matter. It is given exactly (without any linear approximation) by:

$$1 + \delta = \frac{\rho_m}{\bar{\rho}_m} = \frac{M}{\frac{4}{3}\pi R^3} \frac{1}{\bar{\rho}_m}. \quad (4.6)$$

Since $\bar{\rho}_m = \rho_c \Omega_m / a^3$ (where by ρ_c and Ω_m we mean these quantities today; see Eq. (2.37)), the definition of the critical density in Eq. (2.24) yields

$$1 + \delta = \frac{2GM}{\Omega_m H_0^2} \frac{a^3}{R^3} \equiv \lambda \frac{a^3}{R^3}, \quad (4.7)$$

where the final relation defines the constant λ .

In order to find an evolution equation for δ , we take its time derivatives. First note that

$$\frac{\dot{\delta}}{1 + \delta} = \frac{d}{dt} \log(1 + \delta) = 3 \left(\frac{d}{dt} \log a - \frac{d}{dt} \log R \right) = 3 \left(\frac{\dot{a}}{a} - \frac{\dot{R}}{R} \right). \quad (4.8)$$

Taking the derivative of this result gives

$$\frac{\ddot{\delta}}{1 + \delta} - \frac{\dot{\delta}^2}{(1 + \delta)^2} = 3 \left(\frac{\ddot{a}}{a} - \frac{\dot{a}^2}{a^2} - \frac{\ddot{R}}{R} + \frac{\dot{R}^2}{R^2} \right).$$

We now use the acceleration equations [Eq. (4.4) and Eq. (4.5)] to write this as

$$3 \left[-\frac{4}{3} \pi G \bar{\rho}_m + \frac{GM}{R^2} + \left(\frac{\dot{R}}{R} - \frac{\dot{a}}{a} \right) \times \left(\frac{\dot{R}}{R} + \frac{\dot{a}}{a} \right) \right].$$

The expressions for δ and its derivative [Eq. (4.6) and Eq. (4.8)] turn this into

$$3 \left\{ \frac{4}{3} \pi G \bar{\rho}_m [-1 + (1 + \delta)] + \left(-\frac{1}{3} \frac{\dot{\delta}}{1 + \delta} \right) \times \left(-\frac{1}{3} \frac{\dot{\delta}}{1 + \delta} + 2 \frac{\dot{a}}{a} \right) \right\}$$

The final result is thus

$$\ddot{\delta} = 4\pi G \bar{\rho}_m \delta (1 + \delta) - 2 \frac{\dot{a}}{a} \dot{\delta} + \frac{4}{3} \frac{\dot{\delta}^2}{1 + \delta}, \quad (4.9)$$

where the last term on the right-hand side came from adding two such terms, with coefficients 1 and 1/3.

The just-derived equation gives the exact second derivative of δ , valid even when δ is large (i.e. non-linear). However, in cosmology we are often interested in small perturbations, especially in the early Universe, before gravity had time to amplify the tiny initial fluctuations seen in the CMB. Thus, of particular importance is the same relation but where we only keep terms to linear (i.e. first) order in δ . A linear spherical perturbation ($\delta \ll 1$) thus evolves according to

$$\ddot{\delta} = 4\pi G \bar{\rho}_m \delta - 2 \frac{\dot{a}}{a} \dot{\delta}. \quad (4.10)$$

The first term on the right-hand side represents the gravitational forcing (or driving force), whereby high density ($\delta > 0$) tends to increase δ even further (by producing a positive $\ddot{\delta}$). The second term represents Hubble damping, whereby the cosmic

expansion tends to suppress fluctuations (by producing a negative $\ddot{\delta}$); this is physically related to the redshifting of peculiar velocities (Sec. 2.4).

4.1.3. Examples of linear perturbation growth

While we have derived the evolution equation of linear perturbations [Eq. (4.10)] in the spherical case, we show later in this chapter that this equation is correct also in the general, non-spherical case (for pressureless adiabatic modes). Thus, we can use it together with some simple cosmological limits in order to begin to understand the cosmic history of the growth of linear perturbations. We note that since we have a second order, ordinary differential equation, we expect two linearly-independent solutions. They are often denoted δ_+ and δ_- , and referred to as the “growing mode” and “decaying mode”, respectively (since often one of them grows with time and the other declines).

No expansion: When $\dot{a} = 0$, $\bar{\rho}_m$ is constant in time, and the equation is $\ddot{\delta} = 4\pi G\bar{\rho}_m\delta$. The solutions are exponential growth and decay: $\delta_{\pm} \propto \exp(\pm\omega t)$, where $\omega^2 = 4\pi G\bar{\rho}_m$. The characteristic timescale of the exponential growth or decay is of order the dynamical time

$$t_{\text{dyn}} \equiv \frac{1}{\sqrt{G\bar{\rho}_m}}. \quad (4.11)$$

Given initial conditions at time t_i , the full solution is

$$\delta(t) = \delta_+(t_i)e^{\omega(t-t_i)} + \delta_-(t_i)e^{-\omega(t-t_i)}. \quad (4.12)$$

Einstein-de Sitter: In the matter-dominated case with $\Omega_m = 1$, $a \propto t^{2/3}$ [see Sec. 2.3.3], and $\dot{a}/a = H = 2/(3t)$. For the gravitational forcing term we note that $\bar{\rho}_m$ equals the critical density [Eq. (2.24)] in this case, so that $4\pi G\bar{\rho}_m = 3H^2/2 = 2/(3t^2)$. The equation in this case is thus

$$\ddot{\delta} = \frac{2}{3t^2}\delta - \frac{4}{3t}\dot{\delta}. \quad (4.13)$$

If we try a power-law solution, $\delta \propto t^n$, we obtain $3n^2 + n - 2 = 0$. The two solutions are:

$$\delta_+^{\text{EdS}}(t) \propto t^{2/3} \propto a, \quad \delta_-^{\text{EdS}}(t) \propto t^{-1}. \quad (4.14)$$

Given random initial conditions, it is expected that the growing mode will dominate after some time, so $\delta_+ \propto a$ is an important solution that we will use extensively. Note that even when matter dominates, the cosmic expansion suppresses the growth of perturbations, turning it from exponential (in the above no-expansion case) to power-law in time.

Radiation dominated: With $\Omega_r = 1$, $a \propto t^{1/2}$ [Sec. 2.3.3], and $\dot{a}/a = H = 1/(2t)$. We first note that the radiation density is uniform (i.e. non-fluctuating) on sub-horizon scales, since gravity on these scales cannot compete with the high

velocity of the photons (or with their sound speed, which is of order the speed of light). This is why, in general, we only need to consider here the growth of matter fluctuations. Now, when comparing the two terms on the right-hand side of Eq. (4.10), we note that there are two different timescales here: $t \sim 1/H \sim (G\bar{\rho})^{-1/2}$ (where the last relation comes from the Friedmann equation for this case), compared to the dynamical time $t_{\text{dyn}} = 1/\sqrt{G\bar{\rho}_{\text{m}}}$ corresponding to gravitational growth due to matter. Since in this case $\bar{\rho}_{\text{r}} \gg \bar{\rho}_{\text{m}}$, also $t \ll t_{\text{dyn}}$. So, if we want to search for solutions where δ grows significantly during the age of the Universe, i.e. on a timescale t , then for such a solution the ratio between the two terms on the right-hand side of Eq. (4.10) is of order $G\bar{\rho}_{\text{m}} \cdot (\delta/\dot{\delta}) \cdot (a/\dot{a}) \sim (t/t_{\text{dyn}})^2$. Thus, the first term (the driving force) is negligible; note that this is true whenever the component that dominates the cosmic expansion is not matter (and is uniform on the relevant scales). The resulting equation is

$$\ddot{\delta} = -\frac{1}{t}\dot{\delta}. \quad (4.15)$$

We can solve this as a first-order differential equation for $\dot{\delta}$, and then integrate to find the two solutions for δ in a radiation-dominated Universe:

$$\delta_+^{\text{rad}}(t) \propto \log(t/t_i), \quad \delta_-^{\text{rad}}(t) \propto 1. \quad (4.16)$$

These two solutions correspond to weak (logarithmic) growth and no growth, respectively. More generally, when the expansion is not dominated by matter, there is little or no growth of linear perturbations.

4.2. Distribution functions

In order to present linear perturbation theory in the general, non-spherical case, we must deal with the complex motions of large collections of particles. Our approach is to use statistical mechanics, which allows us to follow the overall (macroscopic) properties of the collection (such as the total density and mean velocity of particles at any position) without having to solve for the individual (microscopic) motion of each particle (which is often much harder or impossible).

4.2.1. Quantum statistical mechanics

For classical particles, the distribution function is defined so that the number of particles per phase space volume is $dN = f(\vec{x}, \vec{q}) d^3x d^3q$ [see Sec. 2.3.2], where we use $\vec{q}$ to denote momentum. The same expression is also used in stellar dynamics, where we count stars rather than particles.

To describe various components of the energy density in cosmology, the quantum description of particles is sometimes needed. Thus, we briefly review here basic quantum statistical mechanics.

Consider a quantum particle in a box of length L , i.e. volume $V = L^3$. The Schrödinger equation is then

$$\frac{q^2}{2m}\psi = -\frac{\hbar^2\nabla^2\psi}{2m} = E\psi. \quad (4.17)$$

This is usually written as

$$\nabla^2\psi = -k^2\psi, \quad k^2 \equiv \frac{2mE}{\hbar^2}. \quad (4.18)$$

The 1-D solution is $\psi(x) = A\sin(kx) + B\cos(kx)$, and the boundary conditions $\psi(0) = \psi(L) = 0$ imply that $B = 0$ and $k = n\pi/L$ where $n > 0$ is an integer. In 3-D, separation of variables yields energy eigenstates with

$$E = \frac{q^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2m}(n_x^2 + n_y^2 + n_z^2), \quad (4.19)$$

with n_x, n_y, n_z positive integers (1, 2, 3, ...). The momentum vector is

$$\vec{q} = \frac{\hbar\pi}{L}\vec{n}, \quad (4.20)$$

so the momentum phase space volume is related to n -space as follows:

$$d^3q = \left(\frac{\hbar\pi}{L}\right)^3 d^3n, \quad d^3n = \frac{V}{(\hbar\pi)^3} d^3q. \quad (4.21)$$

This relation can be written as

$$d^3n = \frac{V}{(\hbar\pi)^3} \frac{1}{8} d^3q = \frac{V}{(2\hbar\pi)^3} d^3q, \quad (4.22)$$

where instead of integrating only on positive values of q_x, q_y , and q_z (one octant), we integrate over the full sphere (i.e. all of q -space) and divide by 8 for over-counting. Replacing the volume V with a small volume element d^3x , we thus obtain the expression for counting quantum microstates:

$$\text{Number of quantum microstates : } d^3n = \frac{1}{(2\pi\hbar)^3} d^3x d^3q. \quad (4.23)$$

In quantum statistical mechanics, this expression replaces the phase-space volume element $d^3x d^3q$ of classical statistical mechanics.

More generally, it is necessary to multiply by g , the spin degeneracy factor. With the common particle physics convention of units where $\hbar = c = 1$, the quantum expressions for the number density, energy density, and pressure, are the same as those in the classical case [Eq. (2.27), Eq. (2.28), and Eq. (2.30)], except for an additional factor of $g/(2\pi)^3$. Thus, while we focus on the classical case in what follows, many expressions that we derive below are essentially the same in quantum statistical mechanics.

4.2.2. Fluid frame and stress tensor

We now return to the classical case, corresponding to classical particles or stars. For simplicity, we consider the non-relativistic case, and equal-mass particles. In this case $q = mv$ and $E = mc^2$; often E is simply replaced with m , and then $\rho = mn$ is the mass density (in terms of the number density $n = \int f d^3q$). Now, we derived the formula for the pressure in Sec. 2.3.2, assuming the velocity dispersion is isotropic. When this isotropy is present, this is generally the case only in a particular frame, the *fluid frame*, which moves along with the mean motion of the particles. The momentum components of this frame are

$$\bar{q}_i = \frac{1}{n} \int q_i f d^3q, \quad (4.24)$$

where the index i runs over the number of dimensions. The particle positions in the fluid frame are then

$$\tilde{q}_i \equiv q_i - \bar{q}_i, \quad (4.25)$$

and the pressure is in general defined (even when the random motions are not isotropic) as

$$p = \int \frac{\tilde{q}^2}{3m} f d^3q. \quad (4.26)$$

The pressure is sufficient to describe an isotropic situation, but a more general description uses the *stress tensor*

$$T_{ij} = \int \frac{\tilde{q}_i \tilde{q}_j}{m} f d^3q. \quad (4.27)$$

Removing the pressure component leaves us with the *anisotropic stress tensor*

$$\pi_{ij} = \int \frac{3\tilde{q}_i \tilde{q}_j - \tilde{q}^2 \delta_{ij}}{3m} f d^3q = T_{ij} - p \delta_{ij}, \quad (4.28)$$

where δ_{ij} is a Kronecker delta (equal to unity if $i = j$ and zero otherwise). Note that this tensor is by definition traceless ($\sum_i \pi_{ii} = 0$), while the trace of the stress tensor is $\sum_i T_{ii} = 3p$. A *perfect fluid* has $f = f(\tilde{q})$; in this case there is no anisotropic stress, and $T_{ij} = p \delta_{ij}$. Even more specific is the case of a thermal (Maxwell-Boltzmann) velocity distribution at temperature T , where

$$f \propto \exp[-|\vec{q} - \vec{\bar{q}}|^2 / (2mk_B T)].$$

We will encounter these different cases below.

4.3. The collisionless Boltzmann equation and its moments

In order to derive the equations for the cosmological evolution of matter perturbations, we start from general results in statistical mechanics, which we briefly derive.

4.3.1. *Liouville equation and collisionless Boltzmann equation (CBE)*

In order to help us consider phase space as a genuine six-dimensional coordinate space, we introduce the notation of a six-vector

$$\vec{w} = (\vec{x}, \vec{q}) = (w_1, \dots, w_6). \quad (4.29)$$

Then the trajectory of a particle (or star) is described by

$$d\vec{w}/dt = \dot{\vec{w}} = (\dot{\vec{x}}, \dot{\vec{q}}). \quad (4.30)$$

The distribution of particles, which in general changes with time, is described by the distribution function $f(\vec{w}, t)$. We now consider a six-dimensional volume V that is bounded by the (five-dimensional) area A . Then

$$\frac{\partial}{\partial t} \int_V f dV = - \int_A f \frac{d\vec{w}}{dt} \cdot d\vec{A} = - \int_V \nabla^{(6)} \cdot \left(f \frac{d\vec{w}}{dt} \right) dV. \quad (4.31)$$

Here we have used a number of results generalized from the usual three dimensions (and derived similarly regardless of the number of dimensions). The first equality is the (integral form of the) continuity equation: $\int_V f dV$ is the total number of particles within the phase-space volume V , and (assuming that particles do not appear or disappear, but only move around) this quantity can only change by the flow of particles entering or leaving this volume through its boundary (the direction of $d\vec{A}$ is defined to be normal to the surface element). The second equality is the Divergence theorem (or Stoke's theorem), where $[\nabla^{(6)} \cdot \vec{s}]$ denotes the six-dimensional divergence of a vector $\vec{s}$.

Comparing the left-most and right-most expressions in the above equation yields the differential form of the continuity equation in six dimensions:

$$\frac{\partial f}{\partial t} + \sum_{\alpha=1}^6 \frac{\partial(f\dot{w}_\alpha)}{\partial w_\alpha} = 0. \quad (4.32)$$

Now, assuming the classical Newtonian case,

$$\sum_{\alpha=1}^6 \frac{\partial \dot{w}_\alpha}{\partial w_\alpha} = \sum_{i=1}^3 \left(\frac{\partial v_i}{\partial x_i} + \frac{\partial \dot{q}_i}{\partial q_i} \right).$$

The first term is

$$\frac{\partial v_i}{\partial x_i} = \frac{1}{m} \frac{\partial q_i}{\partial x_i} = 0,$$

since the x_i and q_i are independent coordinates in six-dimensional space (for simplicity we assume here equal-mass particles or stars). The second term is

$$\frac{\partial \dot{q}_i}{\partial q_i} = - \frac{\partial}{\partial q_i} \left(m \frac{\partial \phi}{\partial x_i} \right) = 0,$$

where ϕ is the Newtonian gravitational potential, and in the last step we switched the order of the two partial derivatives and then noted that ϕ may depend on position (and possibly time) but not momentum. Thus, Eq. (4.32) becomes

$$0 = \frac{\partial f}{\partial t} + \sum_{\alpha} \dot{w}_{\alpha} \frac{\partial f}{\partial w_{\alpha}} = \frac{df}{dt}, \quad (4.33)$$

where the second equality uses the definition of the total time derivative of f ; this is sometimes called the Lagrangian derivative or the material/fluid derivative, and expresses the fact that the total change with time of f at the position of a given particle is a combination of the change due to the explicit time-dependence of f and that due to the particle motion to a different six-dimensional position plus the dependence of f on the coordinates w_{α} .

Although we have derived this relation in Cartesian coordinates, the final result (in terms of the total derivative) is valid more generally, in any coordinate system. The meaning of this result is that $f = dN/[d^3x d^3q]$ is constant along a particle trajectory in phase space. It can be thought of as a kind of conservation law for the phase space density. A rough analogy that is sometimes given is to a marathon race. Consider the phase space density around a fixed marathon runner. At the beginning of the race, all the runners are close together, so a given runner is surrounded by runners with many different velocities (i.e. the runners are concentrated in x but spread out in q). After a long time, the runners spread out, and the same initial runner is then surrounded only by those runners that run approximately at his speed (i.e. the runners are spread out in x but concentrated in q , and the overall six-dimensional phase space density is unchanged).

The Liouville equation [Eq. (4.33)], written back in terms of position and momentum, is also called the collisionless Boltzmann equation:

$$\frac{df}{dt} = \left[\frac{\partial}{\partial t} + \frac{d\vec{x}}{dt} \cdot \frac{\partial}{\partial \vec{x}} + \frac{d\vec{q}}{dt} \cdot \frac{\partial}{\partial \vec{q}} \right] f = 0. \quad (4.34)$$

This equation describes the evolution of a collection of particles that move under their collective self-gravity but are otherwise non-interacting (hence “collisionless”).

4.3.2. Moments of the CBE

The CBE is usually too complex to solve directly, as the solution consists of a function of seven variables. Instead, it is common to take its moments, i.e. particular integrals over some of the variables (usually the momentum components), in order to reduce the remaining number of degrees of freedom. It is often possible to solve the resulting equations, at least in some special cases or with some simplifying assumptions.

We consider here the non-relativistic, Newtonian case. The CBE is then

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{x}} - m \vec{\nabla} \phi(\vec{x}, t) \cdot \frac{\partial f}{\partial \vec{q}} = 0. \quad (4.35)$$

We begin by applying $\int d^3q$ to this CBE:

$$\int \frac{\partial f}{\partial t} d^3q + \int v_i \frac{\partial f}{\partial x_i} d^3q + \int (-m) \frac{\partial \phi}{\partial x_i} \frac{\partial f}{\partial q_i} d^3q = 0,$$

where here and in the rest of this section, repeated indices imply summation. In the last term, note that $d^3q = dq_x dq_y dq_z$, and, e.g.

$$\int \frac{\partial f}{\partial q_x} dq_x = 0,$$

assuming physical boundary conditions of $f \rightarrow 0$ at $|q_x| \rightarrow \infty$ (i.e. there are no particles with infinite kinetic energy). Thus, for each $\partial f / \partial q_i$, the integral with respect to dq_i with the same i gives zero, and the entire term vanishes. We now note that $n = \int f d^3q$ [Sec. 2.3.2], and that the average (over the momentum distribution) of any quantity w (at a position $\vec{x}$) is $\bar{w} = [\int w f d^3q] / n$. The partial derivatives with respect to other quantities can be moved outside of the momentum integrals, so we obtain

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i} (n \bar{v}_i) = 0. \quad (4.36)$$

We denote $u_i \equiv \bar{v}_i$, and also note that $\rho = mn$, finally obtaining

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u}) = 0. \quad (4.37)$$

This is the continuity equation, which expresses mass conservation.

The next moment that we take of the CBE in Eq. (4.35) is $\int v_j d^3q$ (separately for each j):

$$\frac{\partial}{\partial t} \int f v_j d^3q + \int v_i v_j \frac{\partial f}{\partial x_i} d^3q - m \frac{\partial \phi}{\partial x_i} \int v_j \frac{\partial f}{\partial q_i} d^3q = 0.$$

In the third term we note that $m v_j = q_j$, and then integrate by parts and note that $\partial q_j / \partial q_i = \delta_{ij}$ (The integrated term vanishes, again assuming that $f \rightarrow 0$ rapidly as $q \rightarrow \infty$). We obtain

$$\frac{\partial}{\partial t} (n u_j) + \frac{\partial}{\partial x_i} (n \overline{v_i v_j}) + \frac{\partial \phi}{\partial x_j} n = 0.$$

To transform the middle term, we note the relation of $\overline{v_i v_j}$ to the same expression but in the fluid frame (given by the mean velocity $\vec{u}$):

$$\overline{(v_i - u_i)(v_j - u_j)} = \overline{v_i v_j} - u_i u_j,$$

so

$$n \overline{v_i v_j} = n u_i u_j + \frac{1}{m} T_{ij},$$

in terms of the stress tensor of Eq. (4.27). We now subtract, from the moment of the CBE that we are considering, u_j times the above continuity equation (in the form

of Eq. (4.36)). Two terms in the resulting equation can be combined as follows:

$$\frac{\partial}{\partial x_i}(n\bar{u}_i\bar{u}_j) - u_j \frac{\partial}{\partial x_i}(n\bar{v}_i) = nu_i \frac{\partial u_j}{\partial x_i}.$$

We then obtain

$$n \frac{\partial u_j}{\partial t} + nu_i \frac{\partial u_j}{\partial x_i} = -n \frac{\partial \phi}{\partial x_j} - \frac{1}{m} \frac{\partial}{\partial x_i} T_{ij}.$$

Dividing by n and using the anisotropic stress tensor of Eq. (4.28) gives

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \vec{\nabla})\vec{u} = -\vec{\nabla}\phi - \frac{1}{\rho}\vec{\nabla}p - \frac{1}{\rho}\vec{\nabla} \cdot \vec{\pi}. \quad (4.38)$$

This is the Euler equation, which expresses momentum conservation. We note that the left-hand side is simply the total derivative of $\vec{u}$ following a trajectory:

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \vec{u} \cdot \vec{\nabla}.$$

To these two moments of the CBE (the continuity and Euler equations), we must add gravity, which in the Newtonian case that we are considering means the Poisson equation:

$$\nabla^2 \phi = 4\pi G \rho. \quad (4.39)$$

In general, the evolution of p and $\vec{\pi}$ depend on still higher moments of the CBE, which follow even more complicated equations. In order to close the set of equations at this point, we require additional assumptions or external information. For example, in the case of a perfect gas, $\vec{\pi} = 0$, and p is given by $p(\rho, s)$ (an equation of state), where s is the specific entropy; it itself follows an evolution equation, such as $ds/dt = 0$ (adiabatic). We also note that

$$\vec{\nabla}p = \left. \frac{\partial p}{\partial \rho} \right|_s \vec{\nabla}\rho + \left. \frac{\partial p}{\partial s} \right|_\rho \vec{\nabla}s. \quad (4.40)$$

When s is spatially uniform (and it remains so under adiabatic evolution), only the first term matters, and it contains the quantity

$$c_s^2 \equiv \left. \frac{\partial p}{\partial \rho} \right|_s, \quad (4.41)$$

where c_s is the (adiabatic) sound speed. For a classical gas, the equation of state is the ideal gas law

$$p = nk_B T = \frac{\rho}{\mu} k_B T, \quad (4.42)$$

where $\mu \equiv \rho/n$ is the *mean molecular weight* (i.e. the mean mass per particle). The specific entropy in this case is $s \propto \ln(p/\rho^\gamma)$, where the adiabatic index is $\gamma = 5/3$ for a monatomic gas including intergalactic gas; it is $7/5$ for gasses consisting of

diatomic molecules, such as air on Earth. Thus, at constant s , $p|_s \propto \rho^\gamma$ and so $c_s^2 = \gamma p / \rho = \gamma k_B T / \mu$. If the gas is isothermal, the result is the same except without the factor of γ .¹ An even simpler case than an ideal gas is cold dark matter, for which $\vec{\pi} = 0$ and $p = 0$, since the velocity dispersion for cold dark matter is negligible at early times. In particular, in the limit of zero dispersion, the particles at any position all move at the same (i.e. fluid) velocity, and the cold dark matter can be pictured like a smooth fluid moving under self-gravity. This limit remains true, though, only until the onset of non-linear collapse, which leads to “shell-mixing”, whereby multiple velocity streams can overlap at a given location. This is discussed further in Sec. 5.3.

An important point to note is that our derivation of the moments in this section used the collisionless Boltzmann equation, and is thus directly applicable to collisionless matter components such as cold dark matter (which is assumed to have interactions that are weak enough to be negligible in analyses of structure formation and galaxy formation). However, in what follows we will want to also analyze the evolution of baryonic gas, in which thermal equilibrium and isotropic pressure are maintained by collisions. Indeed, in what follows we do not directly use the CBE, but only its two moments, the continuity and Euler equations. These equations express the conservation of mass and momentum, respectively, of the particles in a volume of phase space, as we follow them at the fluid velocity. While collisions among gas particles do affect the evolution of the phase-space distribution function f , they conserve mass and momentum, and do not change the center-of-mass motion (and thus the fluid velocity which is averaged over all particles in a given spatial volume). Thus, the continuity and Euler equations remain valid even in the presence of collisions within a gas of particles.

4.4. Eulerian fluid equations in comoving coordinates

We develop here a quasi-Newtonian derivation of perturbation theory. The ultimate justification of the resulting equations, though, requires a full treatment of linear perturbation theory within general relativity (e.g. [1, 2]).

4.4.1. Coordinate transformation

In order to describe the cosmic evolution of non-relativistic matter, we must first consider a general background expansion. In analogy with Eq. (4.5) (though, again,

¹Newton was the first to derive the speed of sound in air from mechanics, and tried to measure it by timing echos at Trinity College of Cambridge University. However, the exposition in his *Principia Mathematica* underestimated the correct speed by $\sim 15\%$ as it incorrectly assumed isothermal conditions (an assumption later corrected by Laplace). Newton’s measurement came out suspiciously low, which may be one more demonstration of the ever-present tension between human nature and absolute scientific integrity; it is important to note, though, that timing a third of a second with a pendulum was not an easy task.

the full justification comes from GR), this requires adding to $d\vec{q}/dt$ the term

$$-\frac{4}{3}m\pi G(\rho + 3p)_{\text{rest}} \vec{r}, \quad (4.43)$$

where from now we use $\vec{r}$ for the (physical) position. We emphasize that the distribution function and quantities derived from it refer only to matter, and do not include other components (which are assumed to be spatially uniform); as a reminder of this, we will write the matter density as ρ_m and not ρ . The next step is to transform the fluid equations (continuity and Euler, plus Poisson), which we have derived in a Newtonian (fixed) coordinate frame, to comoving coordinates as defined in Sec. 2.1.1:

$$\vec{x} = \vec{r}/a, \quad d\tau = dt/a, \quad (4.44)$$

with a corresponding velocity in these coordinates:

$$\vec{v} \equiv \frac{d\vec{x}}{d\tau} = a \frac{d\vec{x}}{dt} = \frac{d\vec{r}}{dt} - H\vec{r} = \vec{u} - H\vec{r}, \quad (4.45)$$

where we used Eq. (2.47). This result shows that $\vec{v}$ is precisely the peculiar velocity.

The transformation to comoving coordinates is really a transformation to variables measured with respect to the mean expanding Universe. When it comes to gravity, instead of the total density we wish to focus on the density perturbation relative to the cosmic mean density, $\Delta\rho_m = \rho_m - \bar{\rho}_m$, or its dimensionless form δ [Eq. (3.1)]. Similarly, we define a peculiar gravitational potential ϕ_{pec} so that $\phi_{\text{pec}} = 0$ for a homogeneous Universe. Indeed, in a uniform Universe there is spherical symmetry, so assuming $\phi = \phi(r)$, the Poisson equation [Eq. (4.39)] (with respect to the proper coordinate $\vec{r}$) is, in spherical coordinates,

$$\nabla_r^2 \phi = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\phi}{dr} \right) = 4\pi G \bar{\rho}_m,$$

where, though we do not explicitly indicate it, $\bar{\rho}_m$ and ϕ may depend on time. The solution (assuming $\phi = 0$ at the origin $r = 0$) is $\phi = 2\pi G \bar{\rho}_m r^2/3$. Thus, in general ϕ_{pec} is defined relative to the mean Universe by

$$\phi_{\text{pec}} = \phi - \frac{2\pi}{3} G \bar{\rho}_m r^2. \quad (4.46)$$

We note that *mathematically* speaking, the force due to the other components in Eq. (4.43) is equivalent to adding to ϕ a term

$$\frac{2\pi}{3} G(\rho + 3p)_{\text{rest}} r^2,$$

since $\vec{\nabla} r^2 = 2\vec{r}$. Thus, the term of Eq. (4.43) does not change any equation derived in the previous section that does not involve ϕ , and it changes the Euler equation

[Eq. (4.38)] by adding, on the right-hand side, the term

$$-\frac{4}{3}\pi G(\rho + 3p)_{\text{rest}} \vec{r}. \quad (4.47)$$

When we transform from coordinates $(\vec{r}, t)$ to $(\vec{x}, \tau)$, we need to also transform the partial derivatives in the fluid equations. Fixed t is the same as fixed τ , so for any function s ,

$$\left. \frac{\partial s}{\partial \vec{x}} \right|_{\tau} = a \left. \frac{\partial s}{\partial \vec{r}} \right|_t. \quad (4.48)$$

A derivative at fixed $\vec{x}$ is more subtle, however. In general,

$$ds = \left. \frac{\partial s}{\partial \vec{r}} \right|_t \cdot d\vec{r} + \left. \frac{\partial s}{\partial t} \right|_{\vec{r}} dt.$$

Since $\vec{r} = a\vec{x}$, at fixed $\vec{x}$ we have $d\vec{r} = \vec{x}da$. Also, in general, $da/d\tau = ada/dt = a^2H$. Thus, dividing ds by $d\tau$ at fixed $\vec{x}$ yields

$$\left. \frac{\partial s}{\partial \tau} \right|_{\vec{x}} = aH\vec{r} \cdot \left. \frac{\partial s}{\partial \vec{r}} \right|_t + a \left. \frac{\partial s}{\partial t} \right|_{\vec{r}}. \quad (4.49)$$

We can also use this in reverse form, as

$$\left. \frac{\partial s}{\partial t} \right|_{\vec{r}} = \frac{1}{a} \left. \frac{\partial s}{\partial \tau} \right|_{\vec{x}} - H\vec{x} \cdot \left. \frac{\partial s}{\partial \vec{x}} \right|_{\tau}. \quad (4.50)$$

In what follows, we use the short-hand notation

$$\vec{\nabla}_r \equiv \left. \frac{\partial}{\partial \vec{r}} \right|_t, \quad \vec{\nabla}_x \equiv \left. \frac{\partial}{\partial \vec{x}} \right|_{\tau}.$$

Also, by $\partial/\partial t$ we mean at constant $\vec{r}$, while $\partial/\partial \tau$ implies at constant $\vec{x}$.

4.4.2. Poisson equation

Since the Poisson equation is linear in ϕ , Eq. (4.39) [which is now correctly understood as referring to ρ_m and not ρ] and Eq. (4.46) together give

$$\nabla_x^2 \phi_{\text{pec}} = a^2 \nabla_r^2 \phi_{\text{pec}} = a^2 \nabla_r^2 \left(\phi - \frac{2\pi}{3} G \bar{\rho}_m r^2 \right) = a^2 (4\pi G \rho_m - 4\pi G \bar{\rho}_m).$$

Thus, the final result is

$$\nabla_x^2 \phi = 4\pi G a^2 \bar{\rho}_m \delta, \quad (4.51)$$

where here and for the rest of this section, we use ϕ to denote the peculiar Newtonian potential ϕ_{pec} (i.e. we drop the subscript).

4.4.3. Continuity equation

We begin with Eq. (4.37), which in the notation of this section is

$$\left. \frac{\partial \rho_m}{\partial t} \right|_{\vec{r}} + \vec{\nabla}_r \cdot (\rho_m \vec{u}) = 0.$$

The first term is

$$\left. \frac{\partial \rho_m}{\partial t} \right|_{\vec{r}} = \left. \frac{\partial}{\partial t} \right|_{\vec{r}} [\bar{\rho}_m (1 + \delta)] = \frac{d\bar{\rho}_m}{dt} (1 + \delta) + \bar{\rho}_m \left[\frac{1}{a} \left. \frac{\partial \delta}{\partial \tau} \right|_{\vec{x}} - H \vec{x} \cdot \left. \frac{\partial \delta}{\partial \vec{x}} \right|_{\tau} \right],$$

where we used Eq. (4.50). The second term in the continuity equation is

$$\begin{aligned} & \frac{1}{a} \vec{\nabla}_x \cdot [\bar{\rho}_m (1 + \delta) (\vec{v} + aH\vec{x})] \\ &= \frac{1}{a} \bar{\rho}_m \vec{\nabla}_x \cdot [(1 + \delta) \vec{v}] + \bar{\rho}_m H \left[\vec{x} \cdot \vec{\nabla}_x \delta + (1 + \delta) \vec{\nabla}_x \cdot \vec{x} \right]. \end{aligned}$$

We now note that $d\bar{\rho}_m/dt = -3\bar{\rho}_m H$ (since $\bar{\rho}_m \propto a^{-3}$), and $\vec{\nabla}_x \cdot \vec{x} = 3$. Combining all terms, and dividing by a factor of $\bar{\rho}_m/a$, yields:

$$\frac{\partial \delta}{\partial \tau} + \vec{\nabla}_x \cdot [(1 + \delta) \vec{v}] = 0. \quad (4.52)$$

4.4.4. Euler equation

The Euler equation [Eq. (4.38)] can be transformed similarly to the continuity equation. Our starting point is the desired left-hand side, which is the comoving version of the total derivative following a trajectory:

$$\frac{d}{d\tau} = \frac{\partial}{\partial \tau} + \vec{v} \cdot \vec{\nabla}_x,$$

applied to the comoving velocity $\vec{v}$. Using Eq. (4.45), Eq. (4.48), and Eq. (4.49), we obtain

$$\frac{\partial \vec{v}}{\partial \tau} + \left(\vec{v} \cdot \vec{\nabla}_x \right) \vec{v} = aH\vec{r} \cdot \vec{\nabla}_r (\vec{u} - H\vec{r}) + a \frac{\partial}{\partial t} (\vec{u} - H\vec{r}) + a \left[(\vec{u} - H\vec{r}) \cdot \vec{\nabla}_r \right] (\vec{u} - H\vec{r}).$$

On the right-hand side, the first term cancels with the second part of the third term, leaving

$$a \frac{\partial \vec{u}}{\partial t} - a\vec{r} \frac{dH}{dt} + a \left(\vec{u} \cdot \vec{\nabla}_r \right) (\vec{u} - H\vec{r}).$$

The last term we split, and then note that $(\vec{u} \cdot \vec{\nabla}_r) \vec{r} = \vec{u}$. We now note that two of the terms we have here equal a times the left-hand side of the Euler equation in proper coordinates [Eq. (4.38)], so we use that equation, with the addition of the term of Eq. (4.47). For simplicity, we assume no anisotropic stress ($\vec{\pi} = 0$). Using also Eq. (4.46), we obtain

$$\left[-\frac{a}{\rho_m} \vec{\nabla}_r p - a \vec{\nabla}_r \left(\phi + \frac{2\pi}{3} G \bar{\rho}_m r^2 \right) - \frac{4}{3} \pi G a (\rho + 3p)_{\text{rest}} \vec{r} \right] - a \vec{r} \frac{dH}{dt} - a H \vec{u},$$

where again we denote ϕ_{pec} simply by ϕ . Now we re-write the $\vec{r}$ gradients as $\vec{x}$ gradients using Eq. (4.48), and the remaining $\vec{u}$ back in terms of $\vec{v}$ using Eq. (4.45). We obtain

$$-a \vec{r} \left\{ \frac{dH}{dt} + H^2 + \frac{4\pi}{3} G [\bar{\rho}_m + (\rho + 3p)_{\text{rest}}] \right\} - a H \vec{v} - \frac{1}{\rho_m} \vec{\nabla}_x p - \vec{\nabla}_x \phi.$$

Now we use the cosmic acceleration equation [Eq. (2.23)] for the mean Universe to see that

$$\frac{dH}{dt} + H^2 = \frac{d}{dt} \left(\frac{da/dt}{a} \right) + \frac{(da/dt)^2}{a^2} = \frac{1}{a} \frac{d^2 a}{dt^2} = -\frac{4\pi G}{3} [\bar{\rho}_m + (\rho + 3p)_{\text{rest}}].$$

Finally, noting that $H = (da/d\tau)/a^2$, the Euler equation in comoving coordinates is

$$\frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \vec{\nabla}_x) \vec{v} = -\frac{1}{a} \frac{da}{d\tau} \vec{v} - \frac{1}{\rho_m} \vec{\nabla}_x p - \vec{\nabla}_x \phi. \quad (4.53)$$

Again, the left-hand side is simply the total derivative following a trajectory, while on the right-hand side, the first term accounts for the redshifting of peculiar velocity ($v \propto 1/a$, Sec. 2.4), the second for the pressure gradient force (when gas pressure is present), and the third for gravity.

With these variables, the mean Universe is the case of $\rho_m = \bar{\rho}_m(t)$, $\delta = \phi = 0$, $\vec{v} = 0$. In the presence of small fluctuations, the rough size of v compared with Hubble expansion can be estimated as follows. From the Euler equation and then the Poisson equation

$$v \sim (\nabla_x \phi) \tau \sim (G a^2 \bar{\rho}_m \delta x) \frac{t}{a} \sim G \bar{\rho}_m \delta r t,$$

while the Hubble expansion is

$$H r \sim (1/t) r.$$

Now, since $t \sim 1/\sqrt{G\bar{\rho}}$, we get

$$\frac{v}{H r} \sim G \bar{\rho}_m \delta t^2 \sim \frac{\bar{\rho}_m}{\bar{\rho}} \delta.$$

In perturbation theory, peculiar velocities are a correction of order δ to the Hubble velocities of cosmic expansion.

4.5. Linear perturbation theory

We now use the equations developed in the previous section to study linear perturbation theory in comoving coordinates. Since we now only use comoving coordinates, in this section $\vec{\nabla}_x$ is simply denoted $\vec{\nabla}$, and $\dot{s}$ means $\partial s / \partial \tau$.

The first step is to linearize the perturbations, i.e. keep only first order in δ and/or $\vec{v}$. Then the Poisson equation in the form of Eq. (4.51) remains unchanged. The continuity equation of Eq. (4.52) simplifies to

$$\dot{\delta} + \vec{\nabla} \cdot \vec{v} = 0, \quad (4.54)$$

and the Euler equation of Eq. (4.53) to

$$\dot{\vec{v}} = -\frac{\dot{a}}{a}\vec{v} - \frac{1}{\bar{\rho}_m}\nabla p - \nabla\phi. \quad (4.55)$$

In the pressure term, the gradient makes it already a first-order term (i.e. there are no gradients if $\delta = 0$ everywhere), so that we were able to change ρ_m to $\bar{\rho}_m$ in this term.

We next consider various classes of solutions to these equations of linear perturbations, but first we note a classification of modes into two types. In general, any vector field (in our case the velocity field $\vec{v}$) can be written as the sum of a longitudinal (or potential) component $\vec{v}_{||}$ and a transverse (or rotational) component $\vec{v}_{\perp}$:

$$\vec{v}(\vec{x}, \tau) = \vec{v}_{||} + \vec{v}_{\perp}, \quad (4.56)$$

where $\vec{\nabla} \times \vec{v}_{||} = \vec{0}$ and $\vec{\nabla} \cdot \vec{v}_{\perp} = 0$. In Fourier space, if we decompose the vector field into waves,

$$\vec{v}(\vec{x}) \sim \sum \vec{v}^{\vec{k}}(\tau) e^{i\vec{k} \cdot \vec{x}},$$

then $\vec{\nabla}$ becomes $i\vec{k}$, and thus we have $\vec{k} \times \vec{v}_{||}^{\vec{k}} = \vec{0}$ and $\vec{k} \cdot \vec{v}_{\perp}^{\vec{k}} = 0$. In words, $\vec{v}_{||}$ is parallel to $\vec{k}$ while $\vec{v}_{\perp}$ is perpendicular to $\vec{k}$, hence the names of these components. We also note that Fourier space makes it easy to see why any vector field can always be decomposed in this way: we take its Fourier transform, divide that into the component in the direction of $\vec{k}$ and the rest, and then transform these two pieces back to real space.

4.5.1. Longitudinal isentropic (“adiabatic”) modes

In general, for our matter component we are interested in either cold dark matter or a baryonic gas. In the latter case, we assume pressure given by an equation of state $p(\rho_m, s)$. Assuming isentropic initial conditions, i.e. $\vec{\nabla}s = 0$ at some t_i , then

adiabatic evolution ($ds/d\tau = 0$) maintains isentropic conditions later on as well. Then in this case the pressure gradient term in the Euler equation is

$$\frac{1}{\bar{\rho}_m} \vec{\nabla} p = \frac{1}{\bar{\rho}_m} \left. \frac{\partial p}{\partial \rho_m} \right|_s \vec{\nabla} \rho_m = \frac{c_s^2}{\bar{\rho}_m} \vec{\nabla} [\bar{\rho}_m(1 + \delta)] = c_s^2 \vec{\nabla} \delta. \quad (4.57)$$

In this term, just as we set ρ_m to $\bar{\rho}_m$ in its form on the left-hand side [see the discussion of Eq. (4.55)], in linear theory we can set c_s^2 to its cosmic mean value in the final form on the right-hand side; in the rest of this section, c_s^2 is to be understood as indicating its spatially-averaged value (which may be time-dependent).

Before continuing, we note that in cosmology the terminology of isentropic modes (more commonly called adiabatic modes) is often used to refer to density fluctuations (such as those generated by the most typical models of cosmic inflation) which are equivalent to adiabatic evolution in time; in other words, the fluctuations are equivalent to some regions being ahead of others by a time Δt (or behind if $\Delta t < 0$), assuming that all density components evolve adiabatically in this extra time. Thus, for each component i (assumed to have a constant density in some region),

$$\Delta \rho_i = \rho_i(t + \Delta t) - \rho_i(t) = \frac{d\rho_i}{dt} \Delta t. \quad (4.58)$$

Thus, the fractional perturbation (where all quantities are evaluated at the unperturbed time t) is

$$\delta_i = \frac{\Delta \rho_i}{\rho_i} = \frac{d\rho_i/dt}{\rho_i} \Delta t = \frac{d \log \rho_i}{d \log t} \left[\frac{\Delta t}{t} \right] = \frac{d \log \rho_i}{d \log a} [H \Delta t], \quad (4.59)$$

where the quantities in square brackets are equal for all components. Thus, for adiabatic fluctuations, the relative density fluctuation is proportional to $d \log \rho_i / d \log a$; in particular, all matter components of the energy density (such as cold dark matter and baryons) have the same δ , while radiation components (such as photons and mass-less neutrinos) have a larger fluctuation by a factor of $4/3$ (since $\rho_r \propto a^{-4}$ while $\rho_m \propto a^{-3}$; see also Sec. 4.8.1). Another way to express this is that in adiabatic fluctuations, the number density ratios among various components are fixed (since all number densities evolve in time in the same way, $\propto a^{-3}$, as long as no particles are created or destroyed). In the opposite case, where number-density ratios of various components of the energy density spatially fluctuate but the total density is unchanged, the fluctuations are called isocurvature.

Now we return to considering an ordinary gas (or cold dark matter). To find the growth of perturbations, we combine the linear equations Eq. (4.54) and Eq. (4.55). We take a partial derivative with respect to τ of the continuity equation, and then use the Euler equation for $\dot{\vec{v}}$, and the Poisson equation in the resulting term $\nabla^2 \phi$.

Using also Eq. (4.57), the result is

$$\ddot{\delta} = -\frac{\dot{a}}{a}\dot{\delta} + c_s^2 \nabla^2 \delta + 4\pi G a^2 \bar{\rho}_m \delta, \quad (4.60)$$

where we used the continuity equation again in the first term on the right-hand side.

If we express δ in Fourier space as

$$\delta(\vec{x}, \tau) = \sum e^{i\vec{k} \cdot \vec{x}} \delta_{\vec{k}}(\tau), \quad (4.61)$$

then the linear perturbation equation becomes

$$\ddot{\delta}_{\vec{k}} = -\frac{\dot{a}}{a}\dot{\delta}_{\vec{k}} + c_s^2(k_J^2 - k^2)\delta_{\vec{k}}, \quad (4.62)$$

where

$$k_J \equiv a \left(\frac{4\pi G \bar{\rho}_m}{c_s^2} \right)^{1/2} \quad (4.63)$$

is known as the *Jeans* wavenumber. Note that k here is comoving, so the corresponding comoving wavelength is $\lambda_J = 2\pi/k_J$, where the physical wavelength is related by $\lambda_{\text{phys}} = a\lambda_{\text{com}}$. The *Jeans mass* is the corresponding mass contained in the initial (unperturbed) sphere of diameter λ_J :

$$M_J = \frac{4\pi}{3} \left(\frac{\lambda_J}{2} \right)^3 \bar{\rho}_m^0, \quad (4.64)$$

where $\bar{\rho}_m^0$ is the present mean density of matter.

An important property of the Fourier decomposition of the perturbations is that it turns the spatial derivatives in Eq. (4.60) to multiplication by factors of k in Eq. (4.62). This means that while the evolution in real space mixes δ at different positions, in Fourier space $\delta_{\vec{k}}$ at each $\vec{k}$ evolves independently from all others. This property of Fourier transforms is essentially a mathematical trick, but it also helps develop physical intuition; it makes it particularly useful to think about perturbation theory in Fourier space, especially in combination with the fact that different $\vec{k}$ modes are statistically independent in a Gaussian random field.

4.5.1.1. $k \gg k_J$

At large k (small scales), the gravitational term $c_s^2 k_J^2$ in Eq. (4.62) is negligible with respect to the pressure gradient term $-c_s^2 k^2$, and the solutions are sound waves. As a simple example, assume that c_s is constant (in both space and time). Then the case of no expansion ($\dot{a} = 0$) yields

$$\delta_{\vec{k}} \propto e^{\pm i k c_s \tau}. \quad (4.65)$$

For instance, $\delta_{\vec{k}} \propto \exp[ik(x \pm c_s \tau)]$ corresponds to a wave traveling with speed c_s in the $\mp x$ direction. With expansion, the EdS case (i.e. matter-dominated with $\Omega = 1$)

has $a \propto \tau^2$, so $\dot{a}/a = 2/\tau$ (note: this is not H since here $\dot{a}$ is the derivative with respect to τ), and the perturbation solutions are

$$\delta_{\vec{k}} \propto \frac{e^{\pm i k c_s \tau}}{k c_s \tau}, \quad (4.66)$$

or instead, the spherical Bessel functions j_0 and y_0 applied to the dimensionless quantity $k c_s \tau$. As always, expansion suppresses growth, in this case causing δ to drop in amplitude with time (instead of only oscillating). We note that for cold dark matter in the limit of zero velocity dispersion, k_J is effectively infinite, and there is no $k \gg k_J$ regime.

4.5.1.2. $k \ll k_J$

At small k , pressure is negligible and the resulting gravity-driven equation is equivalent to the equation that we got in the spherically-symmetric case [Eq. (4.10)], except that here we are using comoving time:

$$\ddot{\delta}_{\vec{k}} = -\frac{\dot{a}}{a} \dot{\delta}_{\vec{k}} + 4\pi G a^2 \bar{\rho}_m \delta_{\vec{k}}. \quad (4.67)$$

The solution, as in Sec. 4.1.3, is a sum of growing and decaying modes:

$$\delta_{\vec{k}} = D_+(\tau) \delta_{\vec{k}}^+ + D_-(\tau) \delta_{\vec{k}}^-, \quad (4.68)$$

where the time dependence of the growing and decaying mode is denoted D_+ and D_- , respectively, while $\delta_{\vec{k}}^+$ and $\delta_{\vec{k}}^-$ are the values of the growing component and the decaying component when $D_+ = D_- = 1$ (they are usually defined to have these values at the present time). In the EdS case, for example, $a \propto \tau^2$, so $aH = \dot{a}/a = 2/\tau$, and the equation is

$$\ddot{\delta}_{\vec{k}} = -\frac{2}{\tau} \dot{\delta}_{\vec{k}} + \frac{6}{\tau^2} \delta_{\vec{k}}. \quad (4.69)$$

The solutions are equivalent to those in Eq. (4.14):

$$D_+^{\text{EdS}} \propto \tau^2 \propto a \propto t^{2/3}, \quad D_-^{\text{EdS}} \propto \tau^{-3} \propto a^{-3/2} \propto t^{-1}. \quad (4.70)$$

Going back to the more general case, when transformed back to real space Eq. (4.68) becomes

$$\delta(\vec{x}, t) = D_+(\tau) \delta_+(\vec{x}) + D_-(\tau) \delta_-(\vec{x}). \quad (4.71)$$

This is a much more powerful result than the mathematically similar solution in the spherical case [Eq. (4.14)]. Here, in full three-dimensional generality (except that small perturbations are assumed), the perturbation pattern (in principle a completely general function of four variables, namely the three spatial coordinates and time) consists of a superposition of two fixed spatial patterns $[\delta_+(\vec{x}) \text{ and } \delta_-(\vec{x})]$, with time-dependent amplitudes. Now, if we assume initial conditions where the

growing and decaying modes have comparable initial values at each position $\vec{x}$, then after some time the growing mode will come to dominate. In this limit,

$$\delta(\vec{x}, t) \approx D_+(\tau) \delta_+(\vec{x}). \quad (4.72)$$

This is an even greater simplification. It means that, in comoving coordinates, the density perturbation field keeps a constant shape, with its amplitude growing with time.

In the longitudinal case, since the velocity field has zero curl, it can be derived from a (proper) velocity potential Φ_v defined so that

$$\vec{v} = -\frac{1}{a} \vec{\nabla} \Phi_v. \quad (4.73)$$

Also, the gravitational acceleration vector $\vec{g}$ is similarly defined in terms of the gravitational potential as

$$\vec{g} \equiv -\frac{1}{a} \vec{\nabla} \phi. \quad (4.74)$$

In the limit of longitudinal perturbations dominated by the growing mode, we can derive various simple relations. The $\vec{v}$ and $\vec{g}$ fields both have zero curl, so let us compare their divergences. From Eq. (4.54),

$$\vec{\nabla} \cdot \vec{v} = -\dot{\delta} = -\frac{\dot{D}_+}{D_+} \delta = -f(\tau) \frac{\dot{a}}{a} \delta,$$

where we used the commonly-defined quantity [3]

$$f(\tau) \equiv \frac{\dot{D}_+/D_+}{\dot{a}/a} = \frac{d \ln D_+}{d \ln a}, \quad (4.75)$$

which equals unity in EdS. Now, Eq. (4.51) can be written as

$$\vec{\nabla} \cdot \vec{g} = -4\pi G a \bar{\rho}_m \delta.$$

Since $\vec{v}$ and $\vec{g}$ both have a divergence that is proportional to $\delta(\vec{x})$, they are proportional to each other. To get a simple form of the proportionality factor, we note from Eq. (2.24) that $4\pi G \bar{\rho}_m = 3\Omega_m H^2/2$, so that

$$\vec{\nabla} \cdot \vec{g} = -\frac{3}{2} H^2 \Omega_m a \delta.$$

Noting also that $\dot{a}/a = aH$, we finally obtain in this limit:

$$\vec{v} = \frac{2}{3} \frac{f}{\Omega_m H} \vec{g}, \quad \Phi_v = \frac{2}{3} \frac{f}{\Omega_m H} \phi. \quad (4.76)$$

Note that one important aspect of this result is that the peculiar velocity is at each point parallel to the local gravitational force (or acceleration).

4.5.2. *Transverse modes*

In general, the curl of the linear Euler equation [Eq. (4.55)] gives:

$$\vec{\nabla} \times \dot{\vec{v}} = -\frac{\dot{a}}{a} \vec{\nabla} \times \vec{v}.$$

This can be rearranged to:

$$\frac{\partial}{\partial \tau} (a \vec{\nabla} \times \vec{v}) = 0.$$

Since the curl determines the transverse component $\vec{v}_\perp$ in Eq. (4.56) (as its divergence vanishes), its time dependence is:

$$\vec{v}_\perp(\vec{x}, \tau) = a^{-1} \vec{v}_\perp(\vec{x}). \quad (4.77)$$

Thus, the transverse component decays over time and becomes more insignificant compared to the longitudinal component (with its growing mode). Also, from the curl of the Euler equation we see that $\vec{v}_\perp$ is not sourced (at linear order) by gravity or pressure (but it can be sourced by anisotropic stress if present).

4.5.3. *GR modes*

We briefly note that there are two other types of modes that arise only within General Relativity, namely vector and tensor perturbations. The Newtonian perturbations that we have thus far considered are referred to as scalar perturbations in this more general context.

Both of the GR types decay for modes on spatial scales below the horizon. Vector perturbations decay like $\vec{v}_\perp$ (i.e. $\propto 1/a$). Tensor perturbations correspond to gravity waves (gravitons), and like photons, their energy density decays as $\rho \propto a^{-4}$. As a result, even if primordial gravitational waves (e.g. from cosmic inflation) contribute substantially to the observed large-scale CMB fluctuations (and there is now a significant limit on that [4]), on sub-horizon scales their amplitude is expected to be too small for direct detection [5].

4.5.4. *No growth*

As we have seen, the only cosmic linear fluctuations that can grow (inside the horizon) are the adiabatic fluctuations of Sec. 4.5.1. Thus, if these fluctuations do not grow significantly, there is no perturbation growth at all.

What drives fluctuation growth is gravity. As seen in Eq. (4.67), gravity is opposed by pressure (which wins on small scales, Sec. 4.5.1.1) and by cosmic expansion (i.e. by the redshifting of peculiar velocity). If expansion wins on all scales, then there is no perturbation growth. The ratio between the gravitational forcing

term and the redshifting term in Eq. (4.67) is roughly

$$\frac{4\pi G a^2 \bar{\rho}_m \delta_{\vec{k}}}{\frac{\dot{a}}{a} \dot{\delta}_{\vec{k}}} \sim \frac{G a^2 \bar{\rho}_m}{a H / \tau}. \quad (4.78)$$

Now we note that

$$\frac{a}{\tau} \sim \frac{a^2}{t} \sim a^2 H,$$

so the ratio is

$$\frac{G a^2 \bar{\rho}_m}{a^2 H^2} \sim \frac{G \bar{\rho}_m}{G \bar{\rho}} = \frac{\bar{\rho}_m}{\bar{\rho}}, \quad (4.79)$$

where we used the Friedmann equation [Eq. (2.21)] and assumed a Universe that is (at least approximately) flat. Thus, whenever $\bar{\rho} \gg \bar{\rho}_m$, the gravitational forcing is negligible compared to the redshift term. This means that if some other component, which does not cluster (on sub-horizon scales), dominates the cosmic density, then matter cannot cluster. Intuitively, gravity causes clustering, but if there is another huge energy density that dominates the cosmic expansion, gravity cannot compete; the expansion is so fast that as soon as gravity produces some peculiar velocity, it redshifts away and does not have time to grow (see the related discussion near the end of Sec. 4.1.3).

It is useful to look at the resulting equation when the redshift term dominates. Eq. (4.67) simply becomes

$$\ddot{\delta}_{\vec{k}} = -\frac{\dot{a}}{a} \dot{\delta}_{\vec{k}}. \quad (4.80)$$

This equation has two solutions for the time dependence of $\delta_{\vec{k}}$. One of them is $\dot{\delta}_{\vec{k}} = 0$ (which corresponds to $\delta = \text{const}$, i.e. frozen fluctuations with no growth). The other solution (which in this case is the growing mode) we can see from the form of the equation, which by now should be quite familiar (e.g. Sec. 4.5.2); it is a redshifting equation for the quantity $\dot{\delta}_{\vec{k}}$, and the solution is

$$\dot{\delta}_{\vec{k}} \propto \frac{1}{a} \implies \delta_{\vec{k}} \propto \int \frac{d\tau}{a} = \int \frac{dt}{a^2}. \quad (4.81)$$

There are two important examples of a universe that is dominated by something other than matter (see Sec. 2.3.3). In a radiation-dominated Universe, $a \propto t^{1/2}$, which gives logarithmic growth. In a Universe dominated by a cosmological constant, a grows exponentially, so that the growing mode converges as $t \rightarrow \infty$ and growth stops. Thus, fluctuations can grow significantly only in a matter-dominated Universe, and otherwise they freeze or, at best, grow logarithmically.

The real Universe has been matter-dominated and well approximated as EdS from just after matter-radiation equality until recent cosmic times. In EdS the growing mode is proportional to $a(t)$ [Sec. 4.5.1], so given the standard normalization of $D(a=1) = 1$, in EdS we would simply have $D(a) = a$. In Λ CDM with our

standard parameters, at high redshift we instead have $D(a) \simeq 1.28a$. In other words, the recent dominance by the cosmological constant in Λ CDM suppresses the linear growth of structure down to the present by a factor of 1.28 compared to a Universe that had continued to follow the EdS model.

4.5.5. The Jeans length

Due to its substantial importance, we further elaborate here on the concept of the Jeans length from Eq. (4.63). This length L corresponds to a balance between pressure and gravity; a perturbation of a region larger than L collapses since its self-gravity is larger than the pressure gradient force, while a perturbation of a smaller region is dissipated by pressure since gravity is too weak to act in time.

We can roughly estimate the Jeans length in various ways. One is to compare timescales. Gravity (due to a matter perturbation) acts on a characteristic timescale of order the dynamical time $t_{\text{dyn}} \sim 1/\sqrt{G\bar{\rho}_{\text{m}}}$, while pressure waves traverse the scale L in a time t_{P} determined by the sound speed, $t_{\text{P}} \sim L/c_{\text{s}}$. Collapse occurs if gravity acts more rapidly, i.e. if $t_{\text{dyn}} < t_{\text{P}}$, which gives

$$L > \frac{c_{\text{s}}}{\sqrt{G\bar{\rho}_{\text{m}}}} = L_{\text{J}}.$$

The quantity on the right-hand-side is the physical Jeans length (up to a factor of order unity), or a times the comoving Jeans wavelength.

Alternatively, we can compare characteristic velocities, where the highest velocity wins. In this case, the velocity corresponding to pressure is simply c_{s} , while that of gravity (the dynamical velocity) is distance over time, $v_{\text{dyn}} = L/t_{\text{dyn}}$. Collapse occurs if $v_{\text{dyn}} > c_{\text{s}}$, which again yields the condition $L > L_{\text{J}}$. We note that while the Jeans length always involves gas pressure, there can be a subtlety in the relevant density $\bar{\rho}_{\text{m}}$. When used in cosmology (for galaxy formation), the density usually refers to the total mass (which is dominated by dark matter), since the gas collapses along with a dark matter fluctuation. On the other hand, when the Jeans mass is used for star formation in gas clouds within a galaxy, the relevant density is usually that of the gas only.

The concept of Jeans length can also be used to (approximately) understand the case of radiation. Photons travel at the speed of light, and their sound speed is also of the same order: $p = \frac{1}{3}\rho$ from Eq. (2.32), combined with Eq. (4.41), yields $c_{\text{s}} = c/\sqrt{3}$. Thus, for photons, $L_{\text{J}} \sim ct_{\text{dyn}}$. Any attempt to grow perturbations starts from the cosmic mean density, for which t_{dyn} is of order the age of the Universe, and then L_{J} is of order the horizon. Thus, perturbations in the radiation on sub-horizon scales cannot grow, and instead undergo acoustic oscillations. This is true for the photon-baryon fluid before cosmic recombination, and these sound waves (acoustic oscillations) are a key to understanding CMB fluctuations.

Another important consideration with regards to the Jeans length is how it changes with time once collapse is initiated. Consider the increase of ρ (of matter)

during the collapse of a fixed mass. Then the size of this mass decreases as $L \propto \rho^{-1/3}$. Meanwhile, the Jeans length changes as well. If we consider an isothermal classical gas, then [see the end of Sec. 4.3.2] the sound speed is constant in time, and $L_J \propto \rho^{-1/2}$. So, assuming that we are considering a collapse, initially $L > L_J$. In the isothermal case, L_J decreases faster than L , so that L remains the larger of the two, and the collapse can continue indefinitely. On the other hand, in the case of an adiabatic collapse with adiabatic index γ , $c_s^2 \propto \rho^{\gamma-1}$ and $L_J \propto \rho^{(\gamma/2)-1}$. In this case, L_J decreases more slowly than L (as long as $\gamma > 4/3$, which includes the monatomic gas value of $5/3$), and at a sufficiently high density L drops to a value equal to L_J , at which point the collapse is halted by pressure gradients. This analysis shows that efficient cooling is essential for gas to reach the extremely high densities that are necessary for star formation.

4.5.6. Super-horizon perturbations

Perturbations of regions of order the horizon or larger require, in principle, a full treatment of general relativistic perturbations. However, we can derive the most important result simply by using the Friedmann equation (which indeed comes from general relativity).² We consider a mean Universe, whose expansion is described by Eq. (2.21):

$$H^2(t) = \frac{8}{3}\pi G\rho,$$

where we assume spatial flatness. Now we consider a small, perturbed region, with a perturbed density ρ_p . Then if we assume the simple case of a uniform spherical region, then (as in Sec. 4.1.2) the perturbed region can be seen as its own Universe, with its own scale factor a_p determined by a Friedmann equation

$$H_p^2(t) = \frac{8}{3}\pi G\rho_p - \frac{k}{a_p^2},$$

where of course the perturbed Universe is not spatially flat. We assume that the Universe in general is dominated by a single component of energy density which has $\rho \propto a^{-n}$, so that

$$\frac{d \log \rho}{dt} = -n \frac{d \log a}{dt} = -nH.$$

Similarly, for the perturbed Universe,

$$\frac{d \log \rho_p}{dt} = -nH_p,$$

²This derivation is based on the beginning of Sec. 5.3 in [1]. However, the derivation in [1] appears to be incorrect since it assumes that $H_p = H$, in our notation. Note though that a different derivation is given later in the same section in [1].

but also $\rho_p \equiv \rho(1 + \delta)$ by the definition of δ , so that

$$\frac{d \log \rho_p}{dt} = \frac{d \log \rho}{dt} + \frac{d \log(1 + \delta)}{dt} \simeq -nH + \dot{\delta},$$

where we simplified the last term to linear order in δ . Thus, $-nH_p = -nH + \dot{\delta}$, which implies

$$H_p^2 = \left(H - \frac{1}{n} \dot{\delta} \right)^2 \simeq H^2 - \frac{2}{n} H \dot{\delta},$$

again to first order. On the other hand, substituting the Friedmann equation for the mean universe into that of the perturbed region gives

$$H_p^2 = H^2(1 + \delta) - \frac{k}{a^2}.$$

In the last term, we changed a_p to a , as k is already a first-order quantity (since $k = 0$ for the mean universe).

Combining the two expressions for H_p^2 finally yields

$$-\frac{2}{n} H \dot{\delta} = H^2 \delta - \frac{k}{a^2}. \quad (4.82)$$

This is a first-order ordinary differential equation for δ . To see if the solution is a power law in time, we first note that the scale factor is a power law in time, as seen from $t \propto (G\rho)^{-1/2} \propto a^{n/2}$, or more rigorously from Eq. (2.35). Now, $H \propto 1/t$, so that the δ and $\dot{\delta}$ terms will have the same power. In order to get the same power in the last (curvature) term, we must have

$$\delta \propto \frac{1}{H^2 a^2} \propto \frac{1}{\rho a^2} \propto a^{n-2}. \quad (4.83)$$

In particular, for $n = 3$ (matter-dominated), $\delta \propto a$, while $n = 4$ (radiation-dominated) gives $\delta \propto a^2$. Inflation is the case of a constant ρ in time (dominated by a constant energy density, as in the case of a cosmological constant), giving $\delta \propto a^{-2}$.

Actually, super-horizon perturbations are difficult to interpret physically, since they cannot be directly measured. Thus, their evolution depends on a choice of gauge within general relativity. In the conformal Newtonian gauge the perturbations are constant outside the horizon (referred to as “frozen”), while our calculation corresponds to the evolution in the synchronous gauge [6]. What matters is the physical (and gauge-invariant) question of the relation between the perturbation size when it leaves the horizon and the size when it comes back in. This can be calculated in any gauge, so in what follows we use these results from the synchronous gauge.

4.6. Cosmic history of perturbations

Given the results derived above, we can now follow the evolution of perturbations throughout cosmic history. Here we derive the approximate evolution, neglecting small corrections such as order unity numerical factors, logarithmic terms, and the relatively short transition periods between different regimes of the cosmic expansion. A key idea in the analysis is that since linear perturbations evolve via equations that are linear in δ , a Fourier decomposition separates out various modes. The amplitude of each mode of a given comoving wavelength λ evolves independently (see the discussion just before Sec. 4.5.1.1). A second key idea is the division of the evolution to sub-horizon and super-horizon stages. To facilitate this division, we note that the comoving horizon (in $c = 1$ units) is [Eq. (2.11)]

$$\tau = \int \frac{da}{a^2 H} \sim \frac{1}{aH},$$

where here we are interested in the largest comoving scale of causal interactions during a given expansion regime, e.g. during a doubling of a (this is different from the usual definition of τ in which the integration starts at the Big Bang and includes all expansion regimes up to some final a). Comparing a perturbation's scale to the horizon means comparing λ to this τ . This is also (approximately) equivalent to comparing the physical scale $\lambda_{\text{phys}} = a\lambda$ to H^{-1} (the Hubble radius).

Consider a given λ . During inflation, $\tau \sim 1/(aH_{\text{inf}})$ declines exponentially with time, since the Hubble constant H_{inf} is fixed in time while the universe expands exponentially. Initially, a is very small and $\tau \gg \lambda$. The perturbation leaves the horizon during inflation when $\lambda \sim 1/(aH_{\text{inf}})$, i.e. $\lambda_{\text{phys}} \sim H_{\text{inf}}^{-1}$, and the scale factor corresponding to exiting the horizon is

$$a_{\text{out}} \sim \frac{1}{\lambda H_{\text{inf}}}. \quad (4.84)$$

We assume that the inflationary period is long enough that all modes of interest exit the horizon during inflation.

The scaling of the size of the perturbations from inflation can be estimated based on Heisenberg's uncertainty principle. Causality (i.e. the inability to communicate faster than the speed of light) implies that the time at which a perturbation leaves the horizon is uncertain by the time needed to transverse this horizon at the speed of light: $\Delta t \sim H_{\text{inf}}^{-1}$. Now, from $\Delta E \Delta t \sim \hbar$, there is an energy uncertainty of $\Delta E \sim \hbar H_{\text{inf}}$. The total energy within the horizon is $E \sim \rho [H_{\text{inf}}^{-1}]^3$, so that the perturbation $\Delta E/E$ is approximately constant in time during inflation. In other words, different λ modes exit the horizon during inflation at different times (i.e. different values of a), but the relative perturbations that they carry are all approximately the same since $\Delta E/E \sim \Delta \rho/\rho$ only depends on quantities that are constant during inflation. This result can be summarized with the phrase *constant δ initial conditions from inflation*. Detailed derivations of this result use quantum field theory [7, 8].

When inflation ends at a_{end} , the Universe enters the radiation-dominated era. From Eq. (2.36), τ increases with a as long as $n > 2$ in $\rho \propto a^{-n}$ (i.e. $w > -1/3$ in $p = w\rho$). In the radiation-dominated era, $\tau \propto a$, and modes that exited the horizon during inflation begin to re-enter the horizon. Also $H \propto 1/t \propto a^{-2}$ during radiation-dominated expansion, so at a given a during this era, the Hubble constant is

$$\frac{H}{H_{\text{inf}}} \sim \left(\frac{a}{a_{\text{end}}} \right)^{-2}.$$

Therefore, the scale factor a_{in} when mode λ re-enters the horizon is given by

$$\lambda \sim \tau \sim \frac{1}{aH} \sim \frac{1}{aH_{\text{inf}}} \left(\frac{a}{a_{\text{end}}} \right)^2,$$

which yields

$$a_{\text{in}} \sim \lambda H_{\text{inf}} a_{\text{end}}^2. \quad (4.85)$$

How does the perturbation amplitude change between exiting and re-entering the horizon? Including the evolution during inflation and then during the radiation-dominated era until re-entry [using Eq. (4.83) for the synchronous gauge outside the horizon],

$$\frac{\delta_{\text{in}}}{\delta_{\text{out}}} \sim \left(\frac{a_{\text{end}}}{a_{\text{out}}} \right)^{-2} \left(\frac{a_{\text{in}}}{a_{\text{end}}} \right)^2 \sim \frac{a_{\text{out}}^2 a_{\text{in}}^2}{a_{\text{end}}^4} \sim 1, \quad (4.86)$$

where we used the above results for the key values of the scale factor. Thus, the perturbation at re-entry has the same size as it did when it exited (consistent with the conformal Newtonian gauge in which the perturbations are simply frozen outside the horizon [6]).

Up until this point, we have followed each mode λ separately, but we now consider all the modes at the same cosmic time. Specifically, at matter-radiation equality, we separate two regimes, based on λ_{eq} , the scale that is just entering the horizon at equality. Modes with $\lambda < \lambda_{\text{eq}}$ entered the horizon before equality, so since there is no significant sub-horizon growth during the radiation-dominated era, their amplitude at equality is

$$\lambda < \lambda_{\text{eq}} : \quad \delta_{\text{eq}} \sim \delta_{\text{in}} \sim \delta_{\text{out}}. \quad (4.87)$$

Modes with $\lambda > \lambda_{\text{eq}}$ have not yet re-entered by equality, so their super-horizon evolution during inflation and then during the radiation-dominated era yields

$$\frac{\delta_{\text{eq}}}{\delta_{\text{out}}} \sim \left(\frac{a_{\text{end}}}{a_{\text{out}}} \right)^{-2} \left(\frac{a_{\text{eq}}}{a_{\text{end}}} \right)^2 \propto a_{\text{out}}^2 \propto \lambda^{-2},$$

where we kept only the scaling with λ . Matching this case with the $\lambda < \lambda_{\text{eq}}$ case at $\lambda = \lambda_{\text{eq}}$, we obtain

$$\lambda > \lambda_{\text{eq}} : \quad \delta_{\text{eq}} \sim \delta_{\text{out}} \left(\frac{\lambda}{\lambda_{\text{eq}}} \right)^{-2}. \quad (4.88)$$

During the matter-dominated era, $\delta \propto a$, both for sub-horizon modes (this is the EdS growing mode) and for super-horizon modes [Eq. (4.83)]. Thus, the relative amplitudes of the various modes remain the same after matter-radiation equality, and the overall normalization simply grows.

We note an important fact about modes that re-enter the horizon during the matter-dominated era, i.e. $\lambda > \lambda_{\text{eq}}$. In this era, $a \propto \tau^2$ so entrance occurs when $\lambda \sim \tau \propto a_{\text{in}}^{1/2}$. To find the amplitude, we combine the evolution until equality with the evolution afterwards, during the matter-dominated era, to find

$$\frac{\delta_{\text{in}}}{\delta_{\text{out}}} \propto \lambda^{-2} \frac{a_{\text{in}}}{a_{\text{eq}}} \propto 1, \quad (4.89)$$

where we kept only the dependence on λ . Matching this case with $\lambda < \lambda_{\text{eq}}$ at the boundary, we conclude that $\delta_{\text{in}} \sim \delta_{\text{out}}$ (i.e. the modes are effectively frozen during their time outside the horizon) for all modes, regardless of when they re-enter the horizon.

We can make interesting inferences from the observation that all modes have approximately the same δ when they exit the horizon during inflation, and also the perturbation size is the same at horizon re-entry. Then this universal perturbation size equals the δ of perturbations currently re-entering the horizon, i.e. the δ of perturbations on the scale of the horizon at present. This corresponds roughly to the perturbations of $\sim 10^{-5}$ first detected in the cosmic microwave background by the COBE satellite [9]. We can also estimate the size of perturbations needed to form galaxies. All galaxies formed from perturbations on scales small enough to have re-entered the horizon during the radiation-dominated era (see the next section). Thus, these perturbations barely grew (logarithmically) until equality, and then have grown roughly in proportion to the scale factor ever since. To form galaxies, these perturbations must have become non-linear (i.e. of order unity) by the present, so they must have started at a size of $1/a_{\text{eq}} \sim 3 \times 10^{-4}$. Compared to these rough estimates, detailed calculations include various factors that we have neglected (numerical factors of a few, logarithmic terms, plus the weak scale dependence of δ from inflation).

4.7. The power spectrum

By definition, $\langle \delta \rangle = 0$, while the contribution of each mode to the variance of δ is $k^3 P(k)/(2\pi^2)$ [Eq. (3.41)]. Interpreting the perturbation amplitude in the previous section as the square root of this (i.e. the standard deviation of δ contributed by

modes within a fixed $\Delta \ln k$ about k), we find a power spectrum shape, at equality or at any later time,³ of

$$P(k) \propto \begin{cases} k & \text{if } k < k_{\text{eq}} \\ k^{-3} & \text{if } k > k_{\text{eq}}, \end{cases} \quad (4.90)$$

corresponding to a variance

$$P(k)k^3 \propto \begin{cases} k^4 & \text{if } k < k_{\text{eq}} \\ 1 & \text{if } k > k_{\text{eq}}. \end{cases} \quad (4.91)$$

More generally, the original power spectrum from inflation may have a somewhat different power law n , so that the above cosmic history gives a power spectrum today of:

$$P(k) \propto \begin{cases} k^n & \text{if } k < k_{\text{eq}} \\ k^{n-4} & \text{if } k > k_{\text{eq}}. \end{cases} \quad (4.92)$$

There are some immediate constraints on n . Large-scale homogeneity implies that $k^3 P(k) \rightarrow 0$ as $k \rightarrow 0$, so that $n > -3$. Also, $k^3 P(k)$ cannot continue to rise with k as $k \rightarrow \infty$ (i.e. n cannot be much above 1), as it would diverge and lead to the early formation of large numbers of primordial black holes. In practice, current observations [10] imply that n is close to (and slightly below) unity, where the $n = 1$ case is known as the Harrison–Zel’dovich spectrum.

The break in the slope occurs at $\lambda_{\text{eq}} \sim c/(aH)$ (where we reinserted the speed of light). Given the scale factor at equality from Eq. (2.57),

$$\lambda_{\text{eq}} \sim \frac{1}{a_{\text{eq}} H_0 \sqrt{2\Omega_r/a_{\text{eq}}^4}} = 97 \left(\frac{\Omega_m h^2}{0.141} \right)^{-1} \text{ Mpc}, \quad (4.93)$$

corresponding to $k_{\text{eq}}^{-1} \sim 16 \text{ Mpc}$ for $\Omega_m h^2 = 0.141$. From Eq. (4.2), a region of diameter λ_{eq} corresponds to a mass scale of $\sim 10^{16} M_\odot$, which is larger than any virialized object in the Universe.

The potential, from the Poisson equation, satisfies $\nabla^2 \phi \propto \delta$, which in Fourier space is $k^2 \phi_k \propto \delta_k$. Thus, the power spectrum is $P_\phi \propto k^{-4} P_\delta$, with corresponding variance (assuming the Harrison–Zel’dovich spectrum)

$$\left(\frac{\Delta \phi}{\phi} \right)^2 \sim k^3 P_\phi \propto \begin{cases} 1 & \text{if } k < k_{\text{eq}} \\ k^{-4} & \text{if } k > k_{\text{eq}}. \end{cases} \quad (4.94)$$

Standard models of cosmic inflation predict a Gaussian random field of isentropic (adiabatic) density fluctuations (see Sec. 4.5.1), and, possibly, significant tensor fluctuations as well. The theory of cosmic inflation has had many successes

³where the amplitude of super-horizon modes is measured in the synchronous gauge.

and has been enormously influential. Proponents point out that since it was first proposed in 1981 [11], many of its basic predictions have been borne out by later observations, including precise flatness, and both Gaussian and adiabatic fluctuations. In addition, while not an example of a prediction, inflationary expansion in a universe effectively dominated by a cosmological constant was a highly novel concept, which was proposed well before observations showed that this is the case in the *present* universe. Critics, however, note that questions about the end of inflation continue to plague the theory, with possible outcomes such as eternal inflation weakening the ability to make clear predictions, while a smoking gun for inflation (such as primordial gravitational waves) has not been seen [4]; alternative ideas have been proposed, including a cyclic universe [12].

4.8. Baryons

In this section we consider a number of different processes and scales related to the evolution of baryons and their perturbations. To begin with, we note a useful number: the cosmic mean (physical) number density of hydrogen (including both neutral and ionized forms) is

$$n_{\text{H}}(z) = 1.90 \times 10^{-7} \left(\frac{\Omega_{\text{b}} h^2}{0.0222} \right) (1+z)^3 \text{ cm}^{-3}, \quad (4.95)$$

assuming that 76% of the baryon mass density is in hydrogen. The number density of helium is smaller by a factor of 12.7 (assuming a helium mass fraction of 24%).

4.8.1. The baryon-photon fluid

At cosmic recombination, protons and electrons recombine into hydrogen atoms. Now, the ionization energy of hydrogen (one Rydberg) is 13.6 eV, which corresponds to a temperature of $\sim 160,000$ K. However, recombination occurs at a much lower temperature of ~ 3000 K, which, given the present CMB temperature of 2.725 K, corresponds to a redshift $z \sim 1100$. In terms of statistical mechanics, this lower temperature is a result of the competition between low energy and maximum entropy. While the recombined atom is the lowest-energy state, the free electron and proton have much higher entropy, and this can compensate for a large Boltzmann factor that disfavors the higher-energy state when the temperature is low.

As long as the atoms are ionized, the baryons and photons are dynamically coupled, and move together. Photons interact furiously with the free electrons through Compton scattering in the non-relativistic limit ($kT \ll m_e c^2$); it is also called Thomson scattering in this limit. Meanwhile, the electrons carry the ions with them due to Coulomb interactions. The rates of all these interactions are so high that to a good approximation the (ordinary) matter and photons can be treated as a single fluid, the *baryon-photon fluid*.

As noted before, the sound speed of radiation is $c/\sqrt{3}$. In the case of the baryon-photon fluid, the photons essentially carry the baryons with them, and this slows down the pressure waves somewhat. The resulting speed of sound can be estimated as follows. Consider the adiabatic evolution of a region containing a fixed number of baryons, which are moving together with photons. This combined fluid has a density $\rho = \rho_\gamma + \rho_b$ and a pressure $p = \rho_\gamma/3$ (since the baryonic pressure is negligible compared to that of the radiation). Also, the entropy density is $s \propto T_\gamma^3$ (since the entropy, like the pressure, is dominated by the photons). Now, assuming that the baryons are neither created nor destroyed, $\rho_b \propto 1/V$, where V is the (changing) volume of the fixed mass of baryons. Thus, the total entropy in the volume V is

$$S \propto T_\gamma^3 V \propto \rho_\gamma^{3/4} / \rho_b. \quad (4.96)$$

Now consider adiabatic evolution, i.e. at constant S : $\rho_b \propto \rho_\gamma^{3/4}$, so $d \log \rho_b = (3/4)d \log \rho_\gamma$ (note the related discussion in Sec. 4.5.1). Thus, changes in the density and pressure are given by $dp = d\rho_\gamma/3$ and

$$d\rho = d\rho_\gamma \left(1 + \frac{3}{4} \frac{\rho_b}{\rho_\gamma} \right).$$

Thus, by definition, the speed of sound is given by

$$c_s^2 = \frac{1}{3 \left(1 + \frac{3}{4} \frac{\rho_b}{\rho_\gamma} \right)}. \quad (4.97)$$

Note also that by definition of a_{eq} ,

$$\frac{\rho_b}{\rho_\gamma} = \frac{a}{a_{\text{eq}}} \frac{\Omega_b}{\Omega_m}. \quad (4.98)$$

Thus, at early times the sound speed is close to $c/\sqrt{3}$, while it later decreases until, around cosmic recombination, it is lower than this value by $\sim 14\%$.

After cosmic recombination, the scattering rate between the photons and baryons drops drastically, leading to a decoupling between them. Here we must distinguish between *cosmic decoupling*, which is when the remaining optical depth seen by a photon drops to unity, and *the end of the drag epoch*, when the optical depth seen by a baryon is unity. Since the number density of photons is much higher, the drag epoch ends somewhat later, at $z_{\text{drag}} \approx 1060$ compared to $z_{\text{dec}} \approx 1090$ (the latter is often denoted z_*) [10]. There is also the much later thermal decoupling (see Sec. 4.8.3 below).

4.8.2. Silk damping

The just-described fluid picture breaks down on small enough scales. Since photon collisions with electrons have a finite rate, the photons diffuse some distance relative to the baryons. This photon diffusion tends to wipe out density fluctuations by

spreading out the photons from over or under-densities. It is known as Silk damping [13]. Its characteristic scale can be estimated as follows.

First we note that the characteristic scale comes out much less than the relevant Jeans scale, which for the baryon-photon fluid is of order the horizon since the sound speed is of order the speed of light (as found in the previous subsection). This means that the effect of gravity on the photon motion can be neglected when estimating the diffusion scale. Now, let l be the proper mean free path of a photon between collisions with electrons. In a time Δt , the average number of collisions is $N = c\Delta t/l$, since the photon moves at the speed of light. Then the root-mean-square comoving distance traversed by the photon is [Eq. (3.34)]

$$\Delta x = \frac{l}{a} \sqrt{2N} = \frac{\sqrt{2c \Delta t l}}{a}.$$

If we cover a cosmologically significant time, then the variance (which for a random walk is the sum of the variances of its portions) is

$$(\Delta x)^2 = \int \frac{2c dt l}{a^2},$$

where both a and l change with time, and the maximum diffusion distance is calculated with an integral from $t = 0$ until cosmic decoupling, when the photons stop scattering. Since the diffusion mostly occurs at temperatures at which the photon energies are far below the electron's rest mass, the collisional cross-section is the fixed (i.e. temperature-independent) Thomson cross-section

$$\sigma_T = 6.65 \times 10^{-29} \text{ m}^2. \quad (4.99)$$

Thus, $l = 1/(n_e \sigma_T) \propto a^3$, so we can write $l = l_{\text{dec}}(a/a_{\text{dec}})^3$. This gives

$$(\Delta x)^2 = \frac{2c l_{\text{dec}}}{a_{\text{dec}}^3} \int_0^{t_{\text{dec}}} a dt.$$

Since decoupling occurs within the matter-dominated era, for a rough estimate we can extrapolate backwards in time using the EdS scaling $t \approx t_{\text{dec}}(a/a_{\text{dec}})^{3/2}$. We obtain

$$\Delta x = \sqrt{\frac{6c l_{\text{dec}} t_{\text{dec}}}{5a_{\text{dec}}^2}}. \quad (4.100)$$

Using the number density of electrons of a fully ionized baryonic plasma, we find $\Delta x \approx 20 \text{ Mpc}$. A cutoff is indeed seen in angular fluctuations corresponding to this scale in the CMB. This cutoff is further enhanced by averaging of the signal over the thickness of the last scattering surface, which has a comparable scale (l_{dec} corresponds to a comoving length of $\sim 1 \text{ Mpc}$ with full ionization, but the last scattering surface is substantially thicker since ionized electrons are disappearing at this time).

If we consider the corresponding baryon drag due to the photons, the relevant mean free path l_e for an electron is given by $n_\gamma \sigma_T l_e = 1$. From Eq. (2.56) and Eq. (4.95), $n_\gamma/n_H \approx 2 \times 10^9$, independent of redshift, and the photon-to-electron ratio at full ionization is the same (up to a small correction from helium). Thus, $l_e \approx l/(2 \times 10^9)$ is very small as long as the gas is ionized.

After decoupling, the baryons no longer move with the photons, and gravity becomes their main driving force, as they begin to fall into the potential wells of the cold dark matter overdensities. However, the baryons are around 1/6 of the matter, which is non-negligible, so they pull on the dark matter and imprint on its density distribution a significant signature of the acoustic oscillations that the baryon-photon plasma had undergone. These are the famous BAOs (baryon acoustic oscillations).

4.8.3. Early history of the Jeans mass

The Jeans length [Sec. 4.5.5] plays a particularly significant role in early cosmic history, specifically in the formation of the first stars. While cold dark matter can collapse and form arbitrarily small halos, the baryons can follow only if a mass is assembled that is above the Jeans mass, so that pressure gradients cannot stop the gravitational collapse of the gas.

Since the Jeans length depends on temperature, for studying the first stars we wish to follow the gas temperature at early times, before the formation of any astrophysical heating sources. While Compton heating of the gas decreases gradually, we can approximate the evolution of the IGM temperature as having a sharp break, where it equals the CMB temperature

$$T_b \approx T_\gamma = 2.725(1+z) \text{ K}$$

down to a transition redshift

$$1+z_t \approx 140 \left(\frac{\Omega_b h^2}{0.0222} \right)^{2/5} \quad (4.101)$$

(this point is also termed thermal decoupling), and decreases adiabatically at $z < z_t$ as for a non-relativistic gas:

$$T_b \approx T_\gamma(z_t) \left(\frac{1+z}{1+z_t} \right)^2. \quad (4.102)$$

From Eq. (4.63) and assuming an ideal monatomic gas, the (comoving) Jeans wavelength equals

$$\lambda_J = 15.7 \sqrt{\frac{T/[70 \text{ K}]}{\mu/[1.22 m_p]} \frac{0.141}{\Omega_m h^2} \frac{60}{1+z}} \text{ kpc}, \quad (4.103)$$

where we used typical numbers corresponding approximately to the first stars, in terms of the redshift [Sec. 11.3], the corresponding IGM temperature (from the just-noted evolution), and μ for neutral gas (see the next subsection). The corresponding Jeans mass from Eq. (4.64) is

$$M_J = 7.94 \times 10^4 \left(\frac{T/[70 \text{ K}]}{\mu/[1.22 m_p]} \frac{60}{1+z} \right)^{3/2} \sqrt{\frac{0.141}{\Omega_m h^2}} M_\odot. \quad (4.104)$$

We note that while the Jeans criterion is calculated for the collapse of gas (i.e. it comes from balancing the pressure gradient force and the gravitational force on gas), the Jeans mass refers to the total mass (including dark matter) in a region of the corresponding size. The Jeans mass is constant at a value of $2.8 \times 10^5 M_\odot$ at high redshift, down to $z \sim z_t$, and then decreases with time $\propto (1+z)^{3/2}$. While the Jeans mass is related to the mass of halos that form the first stars, it does not directly determine this mass, because of considerations related to its evolution over cosmic time, the early history of baryons, and the requirement of gas cooling [Sec. 11.1.2].

4.8.4. Mean molecular weight

We consider here a few example values of the mean molecular weight in cosmology. Since the metallicity is usually quite low in the intergalactic medium, particularly at high redshift, we consider only the simple case of having hydrogen, helium, and free electrons. In general, if, for example, we have three components A , B , and C , with mass per particle m_A and total number of particles (in some fixed volume) N_A (and similarly for B and C), then the mean mass per particle is

$$\mu \equiv \frac{M}{N} = \frac{N_A m_A + N_B m_B + N_C m_C}{N_A + N_B + N_C}. \quad (4.105)$$

We then divide each term by the total mass M , so that each term in the numerator becomes the relative mass contribution of a given component (with a total sum of unity), while the corresponding term in the denominator is the same but divided by the mass per particle of that component. We express this mass per particle in units of the proton mass m_p . We neglect the electron mass compared to a proton, so that electrons are effectively massless and the mass of a hydrogen atom is also m_p (neglecting the small difference). Then we can consider three common cases:

For neutral primordial gas, assuming a helium contribution of 24% by mass:

$$\frac{\mu}{m_p} = \frac{0.76 + 0.24}{0.76 + (0.24/4)} = 1.22. \quad (4.106)$$

For ionized hydrogen with singly ionized helium (corresponding to temperatures approximately in the range of 10,000 – 40,000 K):

$$\frac{\mu}{m_p} = \frac{0.76 + 0.24 + 0}{0.76 + (0.24/4) + [0.76 + (0.24/4)]} = 0.61, \quad (4.107)$$

since $n_e = n_H + n_{He}$ (where we wrote the components in μ in the order of hydrogen, helium, and electrons). For even hotter gas, with fully (i.e. doubly) ionized helium, $n_e = n_H + 2n_{He}$, so

$$\frac{\mu}{m_p} = \frac{0.76 + 0.24 + 0}{0.76 + (0.24/4) + [0.76 + 2 * (0.24/4)]} = 0.59. \quad (4.108)$$

4.8.5. Optical depth due to reionization

As noted in Sec. 4.8.1, the CMB photons scattered often with the free electrons up until cosmic recombination. Much later, ultra-violet photons from stars reionized the inter-galactic medium, at which point the photons could again scatter off the newly-created free electrons. At this stage in cosmic history, densities were much lower, so that only a small fraction of the CMB photons re-scattered. For the simple approximation of sudden reionization at redshift z , we can easily calculate the total optical depth for scattering of a photon between z and the present:

$$\tau_{\text{reion}} = \sigma_T \int_{z'=0}^z n_e(z') c dt, \quad (4.109)$$

in terms of the Thomson cross-section [Eq. (4.99)]. The number density of electrons is the number density of hydrogen [Eq. (4.95)] times a factor $[0.76 + (0.24/4)]/0.76$ assuming reionization with singly-ionized helium (see the previous subsection; we neglect the small effect of the double ionization of helium, which likely occurred at a significantly lower redshift). Now we note that

$$c dt = c \frac{da}{aH} = cH_0^{-1} \frac{da}{a} \left(\frac{\Omega_m}{a^3} + \Omega_\Lambda \right)^{-1/2},$$

where in the last step we neglect the radiation density (which is small at the relevant redshifts). The resulting integral can be done analytically, yielding

$$\tau_{\text{reion}} = 4.03 \times 10^{-3} \left(\frac{\Omega_b/\Omega_m}{0.157} \right) \left(\frac{h}{0.678} \right) \left\{ \sqrt{1 + \Omega_m[(1+z)^3 - 1]} - 1 \right\}. \quad (4.110)$$

Then with our standard cosmological parameters (including $\Omega_m = 0.308$), the latest measured optical depth of 5.5% [14] corresponds to $\tau_{\text{reion}}(z = 7.9)$, i.e. an effective redshift of 7.9 for instantaneous reionization.

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Chapter 5

Non-linear Processes and Dark Matter Halos

In the previous chapter, we followed the development of density perturbations in the limit of small perturbations, to linear order in the relative fluctuation. Gravity, though, increases the size of the perturbations so that eventually they become non-linear (i.e. of order unity or greater) in some regions. In this regime, the simple linear approximation is no longer valid, and a full non-linear calculation of gravity is required. In general, such a calculation is highly complex and can only be attempted numerically. However, in the simple case of spherical symmetry, the evolution can be calculated analytically [1], and the results have proven to be extremely useful in developing intuition, and approximate models, for the formation of galactic halos in the real Universe. We focus here on the formation of halos, which are the hosts of galaxies, but note that on small scales, the power spectrum also changes shape due to the non-linear gravitational growth of perturbations, yielding the *non-linear power spectrum* (e.g. [2]).

5.1. Spherical non-linear collapse

5.1.1. Setup and solution

We restrict ourselves to the simple, EdS case. Then following Sec. 4.1.2, a shell enclosing a fixed mass of matter, M , has a radius R (physical, not comoving) which follows the Newtonian equation of motion

$$\ddot{R} = -\frac{GM}{R^2}. \quad (5.1)$$

The time integral of this equation (after multiplying by $\dot{R}$) is

$$\frac{1}{2}\dot{R}^2 - \frac{GM}{R} = E, \quad (5.2)$$

where we wrote the integration constant as E (which in the Newtonian context is the energy per unit mass of the shell, with the potential energy measured with respect to infinity assuming an empty universe outside the shell). We consider here the case of an expansion that will eventually stop and end in collapse, i.e. $E < 0$.

The solution, written in parametric form, is

$$R = A(1 - \cos \theta), \quad t = B(\theta - \sin \theta). \quad (5.3)$$

In this solution, the Big Bang is represented by $t = 0$ (which corresponds to $\theta = 0$ so also $R = 0$). In order to identify the constants A and B , note that

$$\frac{1}{2}\dot{R}^2 = \frac{1}{2}\frac{A^2}{B^2}\frac{1 + \cos \theta}{1 - \cos \theta} = \frac{1}{2}\frac{A^2}{B^2}\left(-1 + \frac{2}{1 - \cos \theta}\right).$$

According to Eq. (5.2), this must equal

$$E + \frac{GM}{R} = |E|\left[-1 + \frac{GM}{|E|A(1 - \cos \theta)}\right].$$

By matching terms, we find

$$A = \frac{GM}{2|E|}, \quad B = \frac{A}{\sqrt{2|E|}}. \quad (5.4)$$

Note in passing that B , which sets the timescale in the solution for t , is roughly (assuming that the kinetic and potential energy terms are comparable)

$$B \sim \frac{GM}{|E|^{3/2}} \sim \frac{GM}{(GM/R)^{3/2}} = \frac{1}{\sqrt{GM/R^3}} \sim \frac{1}{\sqrt{G\rho}},$$

which is the dynamical time from Eq. (4.11). Next, we note that the perturbation, from Eq. (4.7), is (since we are assuming the EdS case)

$$1 + \delta = \beta \frac{t^2}{R^3}, \quad (5.5)$$

where β is a constant.

5.1.2. Linear limit

We now consider the $\theta \rightarrow 0$ limit, at first to *zeroth* order in δ . In this limit, the parametric solution is

$$R \approx A \frac{\theta^2}{2}, \quad t \approx B \frac{\theta^3}{6},$$

so that $R \propto t^{2/3}$ (corresponding to EdS cosmic expansion at this order), and

$$1 + \delta = \beta \frac{t^2}{R^3} \approx \beta \frac{2B^2}{9A^3}.$$

Setting this to unity at this order yields β . Substituting this constant in Eq. (5.5) then gives us the exact (non-linear) result, valid at all θ :

$$1 + \delta = \frac{9}{2} \frac{(\theta - \sin \theta)^2}{(1 - \cos \theta)^3}. \quad (5.6)$$

By expanding this expression in θ , including two terms each in the numerator and the denominator, we can extract the expression for the linear perturbation:

$$\delta_{\text{lin}} = \frac{3}{20} \theta^2. \quad (5.7)$$

Note that we found $t \propto \theta^3$ above (at early times), so that $\delta_{\text{lin}} \propto t^{2/3}$ is a pure growing mode in EdS (see Sec. 4.1.3 and Sec. 4.5.1). The reason for this is that our solution starts out at the Big Bang, where any decaying mode would extrapolate to infinite magnitude and thus cannot be present.

It is also interesting to consider the perturbation of the Hubble expansion velocity, which by definition is $\dot{R}/R$. The exact spherical solution gives

$$H = \frac{\dot{R}}{R} = \frac{\sqrt{1 + \cos \theta}}{B(1 - \cos \theta)^{3/2}}. \quad (5.8)$$

It is insightful to compare this to the unperturbed EdS value

$$H(\delta = 0) = \frac{2}{3t} = \frac{2}{3B(\theta - \sin \theta)}. \quad (5.9)$$

Expanding these expressions in θ , we find a fractional perturbation

$$\delta_H \equiv \frac{H}{H(\delta = 0)} - 1 = -\frac{1}{3} \delta_{\text{lin}}, \quad (5.10)$$

to linear order. The recession velocity is suppressed by the gravitational pull of a positive perturbation, and for a pure EdS growing mode the velocity perturbation is smaller in amplitude by a factor of $1/3$.

We now define a key concept, the *linearly-extrapolated perturbation*. This is the extrapolation, to non-linear δ , of the evolution in time according to the linear solution for δ . While this linearly-extrapolated magnitude is not accurate in the non-linear regime, it provides a useful reference point. It makes it possible, for example, to compare, at any time, the linearly-extrapolated perturbation to the actual, non-linear, perturbation, and thus clearly identify the effect of non-linear gravitational growth. It is also often useful to talk about the “linear perturbation field” at some late time, rather than only at very early times (when the perturbations really were linear), by referring to the linearly-extrapolated perturbation field (at the present, for example). In the particular case that we are considering in this section, the linearly-extrapolated δ is

$$\delta_L \equiv \frac{3}{20} \left(\frac{6t}{B} \right)^{2/3} = \frac{3}{5} \left(\frac{3}{4} \right)^{2/3} (\theta - \sin \theta)^{2/3}. \quad (5.11)$$

5.1.3. Non-linear stages and the critical density for collapse

A key point in the evolution is *turnaround*, when the expansion is momentarily halted before the ensuing collapse. This milestone is given by $\dot{R} = 0$, corresponding to $\theta_{\text{turn}} = \pi$, $R_{\text{turn}} = 2A$ (the maximum radius), $t_{\text{turn}} = \pi B$, $\delta_{\text{turn}} = (9\pi^2/16 - 1) \approx 4.55$, while $\delta_{L,\text{turn}} = (3/5)[3\pi/4]^{2/3} \approx 1.06$.

The point of *collapse* is the return to $R = 0$, corresponding to $\theta_{\text{col}} = 2\pi$, $\delta_{\text{col}} = \infty$, and $t_{\text{col}} = 2\pi B$. Note that turnaround occurs at half the collapse time, so turnaround corresponds to a δ_L that is smaller than that at collapse by a factor of $2^{2/3}$. Most importantly for later,

$$\delta_{\text{crit}} \equiv \delta_{L,\text{col}} = (3/5)[3\pi/2]^{2/3} \approx 1.686. \quad (5.12)$$

This *critical density* for collapse can be used as a way to estimate the collapse time based on the initial conditions: a region with an initial (linear) overdensity δ_i at time t_i will collapse at time t_{col} given by

$$\delta_i \frac{D_+(t_{\text{col}})}{D_+(t_i)} = \delta_{\text{crit}}.$$

This is only approximate in that it assumes spherical collapse as well as a pure growing mode. If there is a decaying mode component in the initial conditions [Sec. 4.5.1.2] then a standard approach is to include only the growing-mode component δ_i^+ in this estimate, assuming that the decaying-mode component becomes negligible over time. In EdS we thus obtain

$$1 + z_{\text{col}} = \frac{\delta_i^+}{\delta_{\text{crit}}} (1 + z_i). \quad (5.13)$$

For example, for collapse at $1 + z_{\text{col}} = 10$, the initial overdensity at matter-radiation equality ($z \sim 3400$) must have been $\delta_i^+ \sim 5 \times 10^{-3}$. For the very first star, $z_{\text{col}} \sim 65$ [Sec. 11.3], so at equality $\delta_i^+ \sim 3 \times 10^{-2}$.

Finally, we note that although we have followed in this section a single mass shell of enclosed mass M , this also describes the evolution of a *spherical top hat* perturbation. This term refers to a uniform perturbation out to some initial radius R_{max} , containing a total mass M_{max} . All shells containing $0 < M \leq M_{\text{max}}$ have the same value of δ (and thus of θ) at a given time. In terms of the derivation in this section, they all have the same value of B , but different values of $A \propto M^{1/3} \propto R$ at a given time.

In the case of a spherical top hat, the shells all evolve similarly, and collapse to a point together, at the time corresponding to Eq. (5.12). Thus, there is no internal *shell-crossing*, i.e. different shells do not cross each other, and the enclosed mass M stays constant if we follow a fixed thin shell of matter. In addition, there is no external shell-crossing either (i.e. a situation where shells at an initial $R > R_{\text{max}}$ come crashing through the shells at $R < R_{\text{max}}$), as long as the outside shells collapse more slowly, which is the case if the mean enclosed δ within R never rises with R .

This is true, for example, in the simple case of an overdensity surrounded by matter at the cosmic mean density. We also note that after the collapse, if the shells are assumed to bounce back through the origin, then shell crossing does occur, and it results in virialization (discussed in Sec. 5.3 below). In the simple spherical case, this process of *secondary infall* can be solved analytically [3, 4].

5.2. Scaling relations for halos

The results of spherical collapse derived in the previous section are often assumed to give good estimates for properties of real halos; this assumption has stood up well to the test of time, when compared to objects formed in numerical simulations. One particular application of this assumption is the derivation of scaling relations for halos. For simplicity, we assume a scale-free power spectrum, i.e. with a pure power-law dependence. While the real power spectrum in Λ CDM is not so simple, any power spectrum can usually be approximated as a power law over a limited range of scales.

We thus assume a linearly-extrapolated power spectrum of density fluctuations

$$P(k, t) \propto D^2(t) k^n, \quad (5.14)$$

with a scale dependence given by the power n , and time dependence determined by the linear growing mode $D(t)$. For Λ CDM, Eq. (4.90) shows that the actual shape of the power spectrum varies from $n = 1$ at small k to $n = -3$ at large k . More detailed calculations of the intermediate regime find that $n \sim -1$ on the scales corresponding to galaxy clusters, and $n \sim -2$ for large galaxies.

For a given comoving scale R , the variance is

$$\sigma^2(R) = \frac{1}{2\pi^2} \int_0^\infty k^2 dk \tilde{W}^2(k) P(k) \propto D^2 R^{-3-n} \propto D^2 M^{-1-n/3}, \quad (5.15)$$

where the first scaling can be seen by switching variables to $x = kR$ and noting that $\tilde{W}$ is only a function of x , regardless of which window function from Sec. 3.4.2 is used. Some common notations used for this variance are

$$\sigma^2 = \langle \bar{\delta}_R^2 \rangle = \left\langle \left(\frac{\delta\rho}{\rho} \right)^2 \right\rangle = \left\langle \left(\frac{\delta M}{M} \right)^2 \right\rangle. \quad (5.16)$$

The first expression explicitly displays the fact that we have averaged δ over a scale R , the second displays the relative fluctuation in density, and the third is based on the fact that this can also be seen as the relative fluctuation in the mass contained within a fixed comoving radius R .

Next, we note that a given scale becomes non-linear when the corresponding root-mean-square fluctuation $\sigma \sim 1$ (we get similar results if we instead use the

criterion for collapse, which is $\sigma \sim \delta_{\text{crit}}$ from Eq. (5.12)). Then the characteristic non-linear mass M_* scales with time as

$$M_* \propto D^{6/(3+n)} \propto [\text{EdS:}] (1+z)^{-6/(3+n)}, \quad (5.17)$$

where the final expression is the simple result in the EdS case. We conclude that M_* increases with time if $n > -3$. This is the condition for *hierarchical clustering*, in which small halos form first and later accrete more mass and merge into larger ones. The standard Λ CDM model indeed features hierarchical clustering on all scales, although the small galaxies that were common at high redshift formed on scales at which $n \rightarrow -3$; this means that different scales all collapsed at about the same time, i.e. violent *major mergers* (mergers between halos of comparable mass) were common, and galaxies were likely fairly messy and irregular. In models with a sharp cutoff in the power spectrum beyond some value of k (e.g. due to some physical cause such as the large velocity dispersion of warm or hot dark matter, or quantum fuzziness of ultra-light dark matter [5]), the growth of structure is not hierarchical, at least on scales up to the cutoff. In these cases, structure first forms around the cutoff scale, and fragmentation can lead to smaller objects.

For an object that forms at redshift z , the density at formation is

$$\rho_{\text{form}} \propto (1+z)^3 \propto [\text{EdS:}] M_*^{-(3+n)/2}. \quad (5.18)$$

Low-mass halos form early, when the Universe is denser (as are the halos: see the following section). The physical radius is

$$r \propto (M_*/\rho)^{1/3} \propto [\text{EdS:}] M_*^{(5+n)/6}. \quad (5.19)$$

The circular velocity, defined as the velocity of a circular orbit at radius r , and also a measure of the typical infall velocity and of the depth of the potential well, is

$$V_c \sim \sqrt{\frac{GM_*}{r}} \propto \sqrt{M_*^{2/3} \rho^{1/3}} \propto [\text{EdS:}] M_*^{(1-n)/12}. \quad (5.20)$$

In Λ CDM, on all scales $n \leq 1$, so that V_c increases with M_* .

Finally, we note that the correlation function, based on Eq. (3.40), is, for a power-law power spectrum,

$$\xi(r) \propto r^{-(n+3)}.$$

The galaxy correlation function is measured (for large galaxies) to approximately have the power-law shape $\xi \propto r^{-1.8}$, which corresponds to $n = -1.2$. However, this simple relation is *not* considered to be the correct explanation, since the real matter power spectrum is not a power law, and the relation between galaxies and halos is likely quite complicated, involving also the properties of subhalos and satellite galaxies (e.g. [6]).

5.3. Virialization

While the spherical collapse considered in Sec. 5.1 leads to collapse to a point, any realistic collapse does not have precise spherical symmetry. In that case, the mass does not all collapse together, but various mass elements pass near the region of highest density, bounce around, and gradually gather together as the mass located near the center grows. Even if initially the process can be seen as an orderly collapse of roughly-spherical mass shells, at some point the shells cross each other, bounce back and forth multiple times, and give each other gravitational impulses in random directions. This *violent relaxation* process [7] has the effect of changing the ordered collapse, which was characterized by mostly radial infall velocities, to a temperature-like velocity dispersion, with an approximately isotropic distribution of velocities.

Usually a quasi-static equilibrium is reached in some region, where the velocities are isotropic and the overall density profile is not changing much with time. This is what is referred to as a *virialized object*, which satisfies the virial theorem

$$|U| = 2K. \quad (5.21)$$

Here $K > 0$ and $U < 0$ are the total kinetic and potential energy, respectively, of the matter within the virialized (or “collapsed”) object. We defer the proof of the virial theorem to Sec. 6.4. It implies that the total energy is

$$E = U + K = \frac{U}{2} < 0, \quad (5.22)$$

so that the object is gravitationally bound.

To derive the properties of virialized objects, we compare the virialized state to turnaround, and assume energy conservation. For a total mass M , if the total energy at turnaround (when $K = 0$) equals the total energy at virialization, then

$$E = -\frac{GM}{R_{\text{turn}}} = -\frac{GM}{2R_{\text{vir}}},$$

which yields

$$R_{\text{vir}} = \frac{R_{\text{turn}}}{2}. \quad (5.23)$$

We have assumed here the EdS case, since in other cases the contribution of the additional force term of Eq. (4.43) makes things a bit more complicated.

This result implies that the mean enclosed density at virialization is 8 times larger than at turnaround. This density is commonly expressed in terms of the cosmic mean density of matter at the time of virialization. Assuming that this time is well approximated by the collapse time of spherical collapse leads to

$$\frac{\rho_{\text{vir}}}{\bar{\rho}(t_{\text{vir}})} = \frac{8\rho_{\text{turn}}}{\left[\frac{a(t_{\text{vir}})}{a(t_{\text{turn}})}\right]^{-3} \bar{\rho}(t_{\text{turn}})} = \frac{8(1 + \delta_{\text{turn}})}{\left(\frac{t_{\text{col}}}{t_{\text{turn}}}\right)^{-2}} = \frac{8}{1/4} \frac{9\pi^2}{16} = 18\pi^2 \simeq 177.7, \quad (5.24)$$

where we assumed the EdS case and applied from Sec. 5.1.3 both $t_{\text{col}} = 2t_{\text{turn}}$ and the result for δ_{turn} . This is a very important result, namely, that the virial overdensity of halos (in the EdS case) is a fixed factor times the cosmic mean density at virialization; this result also implies that the factor by which the collapse occurred (relative to comoving Hubble flow) in each dimension equals $(18\pi^2)^{1/3} \simeq 5.62$. We note that an important property of spherical collapse in the EdS universe is that both the virial overdensity found here, and the critical density of Eq. (5.12), are fixed numbers independent of the redshift and halo mass; they do vary slightly with redshift in Λ CDM (at low redshift when Λ is non-negligible).

When gas falls into a collapsing halo, shell-mixing results in shock-heating (at what is referred to as the accretion shock or virial shock), and in a collisional thermalization of the kinetic energy. This is the baryonic version of virialization, and it is seen prominently in some simulations [8, 9]. We note, though, that in many galactic halos a cooling instability prevents much of the gas from shocking near the virial radius, and it instead reaches into the halo center in cold streams that trigger star formation [10].

5.4. The Press–Schechter model

A simple analytical model that has become a foundation of theoretical work in galaxy formation was developed by Press & Schechter (1974) [11]. This model for the halo abundance presents a way to connect the initial density field to the abundance by mass of the final, virialized halos. Specifically, the model is based on a few key ideas:

- (1) Gaussian random field: The density perturbation δ is given by an initial Gaussian random field, with a given power spectrum $P(k)$.
- (2) Linear perturbation theory: The growing mode dominates, so that the time dependence of the fluctuations is simply $\delta \propto D_+(t)$.
- (3) Spherical collapse: Formation of a virialized object corresponds to $\delta = \delta_{\text{crit}}$ from Eq. (5.12).

To determine the abundance of halos at a redshift z , in this model we use δ_M , the density field smoothed on a mass scale M , as defined in Sec. 3.4.2, usually with the top hat in real space, and with M translated to a smoothing radius R as in Eq. (4.2). Although the model is based on the initial conditions, it is usually expressed in terms of redshift-zero quantities. Thus, we use the linearly-extrapolated density field, i.e. the initial density field at high redshift extrapolated to the present by simple multiplication by the relative linear growth factor. This is related to the “present power spectrum”, which refers to taking the initial power spectrum and linearly-extrapolating it to the present (i.e. without including non-linear evolution).

The key idea is to assume that for any position $\vec{x}$, $\delta_M(\vec{x}) > \delta_{\text{crit}}$ implies that the mass at the point $\vec{x}$ belongs to a halo of at least mass M . Since δ_M is distributed as

a Gaussian variable with zero mean and standard deviation $\sigma(M)$ [which is determined by Eq. (3.55) with $r = 0$, from the present power spectrum], the probability that δ_M is greater than δ_{crit} is

$$P(\delta_M > \delta_{\text{crit}}) = \int_{\delta_{\text{crit}}}^{\infty} d\delta_M \frac{1}{\sigma(M) \sqrt{2\pi}} \exp\left[-\frac{\delta_M^2}{2\sigma^2(M)}\right] = \frac{1}{2} \operatorname{erfc}\left[\frac{\delta_{\text{crit}}}{\sqrt{2}\sigma(M)}\right]. \quad (5.25)$$

The idea is to identify this probability with the fraction of dark matter particles that are part of collapsed halos of mass greater than M , at redshift 0 (or using the appropriate $\sigma(M)$ at other redshifts). However, there is a problem with this formula. At $M \rightarrow 0$ or $t \rightarrow \infty$, $\sigma(M) \rightarrow \infty$. In this limit (more precisely, when $\sigma(M) \gg \delta_{\text{crit}}$), this probability $P \rightarrow 1/2$. Only half of the mass can ever be assigned to halos in this scheme, since linear fluctuations are symmetric between $+$ and $-$, while only positive fluctuations contribute to $P(\delta_M > \delta_{\text{crit}})$ [Note that for spherical collapse in EdS, the mean universe corresponds to $E = 0$ in Eq. (5.2), so that any positive perturbation leads to an eventual collapse].

The original solution for this dilemma was to correct this by multiplying by an additional factor of two in order to ensure that every particle ends up as part of some halo with $M > 0$. Thus, the fundamental ansatz of the PS model is:

$$F(> M, z) = \operatorname{erfc}\left[\frac{\delta_{\text{crit}}(z)}{\sqrt{2}\sigma(M)}\right], \quad (5.26)$$

where $F(> M, z)$ is the mass fraction contained in halos of mass $> M$ at redshift z . Here we have introduced another common notation, $\delta_{\text{crit}}(z)$. In reality, the threshold δ_{crit} is independent of redshift (as in Eq. (5.12), again assuming the EdS case), while $\sigma(M)$ grows with time with the linear growth factor, i.e.

$$\sigma(M, z) = \sigma(M) \frac{D_+(z)}{D_+(0)}.$$

However, since the mass fraction in halos in the PS model depends only on the ratio between $\sigma(M)$ and δ_{crit} , it has become conventional to use at all redshifts the fixed $\sigma(M)$ at $z = 0$, and preserve the correct ratio versus z by using an effective threshold that rises with redshift:

$$\delta_{\text{crit}}(z) \equiv \frac{1.686}{D_+(z)}, \quad (5.27)$$

where we follow the convention of setting $D_+(0) = 1$. The key ratio

$$\nu_c \equiv \frac{\delta_{\text{crit}}(z)}{\sigma(M)} \quad (5.28)$$

is the number of standard deviations that the critical collapse threshold at z represents for fluctuations on a mass scale M (see Fig. 5.1).

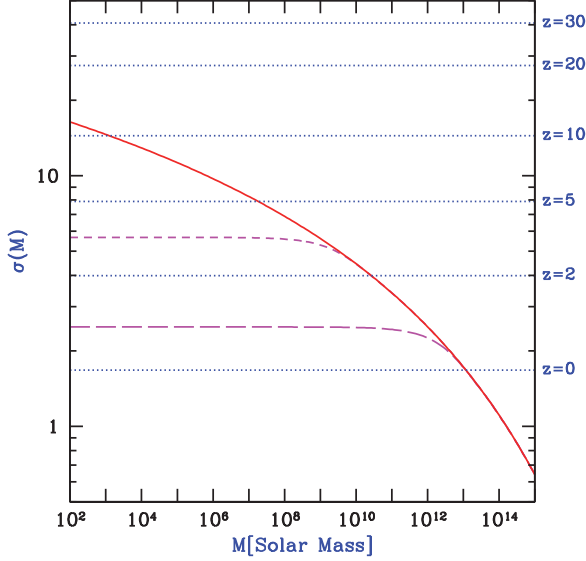


Fig. 5.1. Mass fluctuations and collapse thresholds. The horizontal dotted lines show the value of the extrapolated collapse overdensity $\delta_{\text{crit}}(z)$ at the indicated redshifts. Also shown is the value of $\sigma(M)$ in a Λ CDM model with $\Omega_m = 0.3$ (solid curve), as well as $\sigma(M)$ illustrated for a power spectrum with a cutoff, below a mass $M = 1.7 \times 10^8 M_\odot$ (short-dashed curve) or $M = 1.7 \times 10^{11} M_\odot$ (long-dashed curve). The intersection of the horizontal lines with the other curves indicate, at each redshift z , the mass scale (for each model) at which a 1σ fluctuation is just collapsing at z . From [12].

Given the cumulative mass fraction of the PS model in Eq. (5.26), we can derive the mass distribution function of halos as follows. The comoving mass density (mass per unit volume) in halos within the mass range $M \rightarrow M + dM$ is

$$M dn = \bar{\rho}_m dF,$$

where n is the number of halos per comoving volume, and $\bar{\rho}_m$ is the cosmic mean matter density at $z = 0$. So the halo abundance (or *halo mass function*) is

$$\frac{dn}{dM} = \frac{\bar{\rho}_m}{M} \left| \frac{dS}{dM} \right| f(\delta_{\text{crit}}(z), S), \quad (5.29)$$

where $S = \sigma^2(M)$ is the variance on scale M , and $f(\delta_{\text{crit}}(z), S) = dF/dS$. Thus, $f(\delta_{\text{crit}}(z), S) dS$ is the mass fraction contained at z within halos with mass in the range corresponding to S to $S + dS$; it is possible to use either M or S as the dependent variable. In the Press–Schechter (PS) model,

$$f_{\text{PS}}(\delta_{\text{crit}}(z), S) = \frac{1}{\sqrt{2\pi}} \frac{\nu_c}{S} \exp \left[-\frac{\nu_c^2}{2} \right], \quad (5.30)$$

where we used Eq. (5.28).

The biggest weakness in the derivation of the PS model is probably the ad-hoc factor of two. Bond *et al.* (1991) [13] found a more satisfactory derivation of this correction factor, using a more convincing ansatz. In their derivation, the factor of two originates from the so-called “cloud-in-cloud” problem: For a given mass M , even if δ_M is smaller than $\delta_{\text{crit}}(z)$, it is possible that the corresponding region lies inside a region of some larger mass $M_L > M$, with $\delta_{M_L} > \delta_{\text{crit}}(z)$. In this case, the original region should be counted as belonging to a halo of mass M_L . Bond *et al.* showed that, under certain assumptions, the additional contribution results precisely in a factor of two correction to the halo mass function. We note that this same work was also the basis of substantial further development of the model [14], commonly referred to as the “extended Press–Schechter model”.

The classic PS [11] model has become the basis for the theoretical understanding and modeling of the halo mass function, since it fits fairly well the abundance measured in numerical simulations. In recent decades, big advances in observational cosmology have made even better precision necessary. Particularly important for the second part of this volume is that the PS mass function substantially underestimates the abundance of rare halos (which includes most galactic halos that form at high redshift). The halo mass function of Sheth & Tormen (1999) [15], with modified best-fit parameters [16], fits numerical simulations much more accurately [17]. It is given by:

$$f_{\text{ST}}(\delta_{\text{crit}}(z), S) = A' \frac{\nu}{S} \sqrt{\frac{a'}{2\pi}} \left[1 + \frac{1}{(a'\nu^2)^{q'}} \right] \exp \left[-\frac{a'\nu^2}{2} \right], \quad (5.31)$$

with best-fit parameters $a' = 0.75$ and $q' = 0.3$, and where normalization to unity is ensured by taking $A' = 0.322$. Measurements and fits of the halo mass function continue to be refined [18].

5.5. Mass-radius relations for virialized halos

Given the results we derived in Sec. 5.3 for the properties of virialized halos, we can extend the mass-radius relations for the initial halo mass [Sec. 4.1.1] to the final, virialized state. In particular, for a halo of mass M collapsing at redshift z (assumed high enough for the EdS limit), the physical virial radius is

$$\begin{aligned} R_{\text{phys,vir}} &= \frac{1}{1+z} \frac{R_{\text{com,init}}}{5.62} \\ &= 1.51 \left(\frac{\Omega_m h^2}{0.141} \right)^{-1/3} \left(\frac{M}{10^8 M_\odot} \right)^{1/3} \left(\frac{\Delta_c}{18\pi^2} \right)^{-1/3} \left(\frac{1+z}{10} \right)^{-1} \text{ kpc}. \end{aligned} \quad (5.32)$$

Here we have written the general formula for a final mean halo density equal to Δ_c times the critical density at the collapse redshift. This is $18\pi^2 \simeq 178$ in spherical collapse in EdS [Sec. 5.3]; this theoretical value is slightly modified in Λ CDM, but

conventionally the EdS value (or even the rougher value of 200) is often used to *define* the virial radius r_{vir} and the virial masses of halos in numerical simulations and in analyses of observations.

As noted in Sec. 5.2, another important quantity is the circular velocity

$$\begin{aligned} V_c &= \left(\frac{GM}{r_{\text{vir}}} \right)^{1/2} \\ &= 16.9 \left(\frac{\Omega_m h^2}{0.141} \right)^{1/6} \left(\frac{M}{10^8 M_\odot} \right)^{1/3} \left(\frac{\Delta_c}{18\pi^2} \right)^{1/6} \left(\frac{1+z}{10} \right)^{1/2} \text{ km s}^{-1}. \end{aligned} \quad (5.33)$$

Now, V_c measures the potential depth, and the virial theorem sets the kinetic energy as equal in magnitude to half the potential energy. When gas collapses into the halo, it shocks and its kinetic energy gets converted into random thermal motion. Thus, the characteristic temperature of virialized gas is set by the potential depth. The virial temperature is

$$\begin{aligned} T_{\text{vir}} &= \frac{\mu m_p V_c^2}{2k_B} \\ &= 1.03 \times 10^4 \left(\frac{\Omega_m h^2}{0.141} \right)^{1/3} \left(\frac{\mu}{0.6} \right) \left(\frac{M}{10^8 M_\odot} \right)^{2/3} \left(\frac{\Delta_c}{18\pi^2} \right)^{1/3} \left(\frac{1+z}{10} \right) \text{ K}, \end{aligned} \quad (5.34)$$

where μ is the mean molecular weight in units of the proton mass m_p . We caution that sometimes a different numerical factor is used, in place of the 1/2, in the definition of T_{vir} .

5.6. The galaxy luminosity function

An important quantity that is related to the PS model of Sec. 5.4 is the Schechter luminosity function. Just as the PS model is the simplest analytical formula that describes the halo abundance (as measured in simulations) reasonably well, the Schechter luminosity function is the simplest analytical formula that does so for the luminosity distribution of galaxies (as measured in observational galaxy surveys). In general, if $n_g(L)$ is the total number density (i.e. number per unit volume) of galaxies with luminosity (in some band) above L , then

$$\frac{dn_g(L)}{dL} \equiv \frac{\phi(L/L_\star)}{L_\star}, \quad (5.35)$$

where $L_\star$ is a characteristic galaxy luminosity, and this equation defines the luminosity function ϕ , which has units of number density. The Schechter luminosity

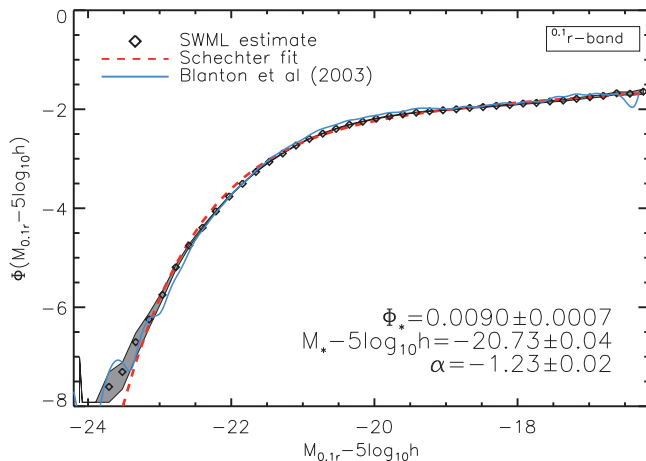


Fig. 5.2. The galaxy luminosity function. We show a recent measurement based on 517,000 galaxies from the Sloan Digital Sky Survey Data Release 6 (points; SWML stands for the Stepwise Maximum Likelihood method, a statistical technique used in the analysis), compared to the best-fit Schechter luminosity function (dashed curve); the thin solid curve shows a previous measurement based on 148,000 galaxies. Instead of luminosity the plot uses the absolute magnitude M (in the r -band shifted to $z = 0.1$), which is a linear function of the logarithm of the luminosity. From [19]

function is

$$\phi_{\text{Schechter}}(x) = \phi_{\star} x^{\alpha} e^{-x}, \quad (5.36)$$

where $\phi_{\star}$ is an overall normalization (with units of number density), and the shape is a power-law (with index α) at low luminosity, with an exponential cutoff at high luminosity. This luminosity function is an excellent match to observed galaxies, even for recent measurements based on large numbers of galaxies (Fig. 5.2).

The Schechter luminosity function was originally inspired by the Press–Schechter model, but the relationship between the two is not thought to be simple. Indeed, we can easily rule out the simplest case, in which we assume a one-to-one relation between halos and galaxies and expect that the two formulas are identical. In order to match the low-luminosity power-law shape of the Schechter luminosity function, we assume a power-law power spectrum as in Eq. (5.14), and compare Eq. (5.29) and Eq. (5.30) to Eq. (5.36). Demanding first that the two exponentials have equal exponents, using Eq. (5.15) we obtain

$$L \propto \nu_c^2 \propto M^{1+n/3}.$$

Thus, the relation between L and M must be a power law. A one-to-one relation between halos and galaxies therefore implies

$$\frac{dn_g}{d\log L} \propto \frac{dn_{\text{halo}}}{d\log M}.$$

We now compare the power-law terms (outside the exponential cutoffs), and demand the same power-law dependence on M ; noting the scaling

$$\left| \frac{dS}{dM} \right| \frac{\nu_c}{S} \propto \frac{1}{\sigma M} \propto M^{-1/2+n/6},$$

we obtain

$$(1 + \alpha) \left(1 + \frac{n}{3} \right) = \left(-\frac{1}{2} + \frac{n}{6} \right),$$

which finally yields

$$\alpha = -\frac{n+9}{2n+6}.$$

Fits to galaxy surveys yield $\alpha \sim -1$, which from this relation corresponds to $n \sim 3$. However, fits of the PS model to the abundance of halos yields $n \sim -2$ for galaxies, which corresponds to $\alpha \sim -3.5$. This utter failure to get reasonable values for both n and α immediately implies that the relation between the halo mass function and the galaxy luminosity function is much more complicated than can be captured by any simplistic model. In reality, both the relationship between halo and galaxy numbers and between a galaxy's luminosity and the host halo mass are believed to be quite complicated and affected by many physical processes. A typical picture of a halo is that it hosts a large central galaxy with some smaller satellites, where the number of satellites goes up to thousands in galaxy clusters, while on the other hand very small halos may not at all host galaxies that formed any stars.

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Chapter 6

Stellar Dynamics and the Virial Theorem

In this chapter and the next one, we temporarily put aside cosmology and the large-scale properties of the Universe, and study the evolution of stellar systems, following [1]. Since stellar collisions are extremely rare and do not affect the overall distribution of stars (except in extreme environments such as globular clusters or galactic centers), we can apply the collisionless Boltzmann equation and related results derived in Chap. 4. The results are also valid for other collisionless systems, and some in particular (such as the virial theorem) are quite important also for cold dark matter halos.

6.1. Collisionless stellar systems

We assume, for simplicity, equal-mass stars (or cold dark matter particles), and begin by re-writing some results that we previously derived, in notation that is more common in stellar dynamics. We use $\vec{x}$ for the position (in fixed coordinates, no comoving ones in this chapter), and go from $\vec{q}$ (momentum) and ρ (mass density) to $\vec{v}$ (velocity) and n (number density). Note that we can easily go between ρ and n if we assume that μ , the mean mass per particle, Then instead of Eq. (2.26), we define the phase-space distribution function by

$$dN = f(\vec{x}, \vec{v}, t) d^3x d^3v . \quad (6.1)$$

The stellar number density [cf. Eq. (2.27)] is

$$n(\vec{x}) = \int f d^3v, \quad (6.2)$$

the mean (fluid) velocity [cf. Eq. (4.24)] is

$$u_i = \bar{v}_i = \frac{1}{n} \int v_i f d^3v, \quad (6.3)$$

and the particle velocities in the fluid frame are $\tilde{v}_i \equiv v_i - \bar{v}_i$. Instead of the stress tensor [Eq. (4.27)], we have the *velocity dispersion tensor*

$$\sigma_{ij}^2 = \frac{1}{n} \int \tilde{v}_i \tilde{v}_j f d^3v. \quad (6.4)$$

The notation σ^2 here reflects the velocity squared units, and component (i, j) of this tensor is simply the mean value (or fluid average) of $\tilde{v}_i \tilde{v}_j$.

The CBE [cf. Eq. (4.34)] is written in the form

$$\frac{df}{dt} = \left[\frac{\partial}{\partial t} + \frac{d\vec{x}}{dt} \cdot \frac{\partial}{\partial \vec{x}} + \frac{d\vec{v}}{dt} \cdot \frac{\partial}{\partial \vec{v}} \right] f = 0. \quad (6.5)$$

Its moments are re-written as follows. The continuity equation [Eq. (4.37)] is written back in terms of number density [Eq. (4.36)]:

$$\frac{\partial n}{\partial t} + \vec{\nabla} \cdot (n\vec{u}) = 0, \quad (6.6)$$

and the Euler equation [Eq. (4.38)] becomes

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \vec{\nabla})\vec{u} = -\vec{\nabla}\phi - \frac{1}{n}\vec{\nabla} \cdot \left(n\vec{\sigma}^2 \right). \quad (6.7)$$

In the context of stellar dynamics, the continuity and Euler equations are together referred to as the *Jeans equations*, in tribute to James Jeans who first applied these equations (originally derived by Maxwell) to stellar systems. As always, we also have the Poisson equation [Eq. (4.39)]; we will use Φ for the gravitational potential since, in what follows, ϕ is reserved for an angular coordinate.

6.2. The collisionless Boltzmann equation in spherical coordinates

In statistical mechanics, it is often difficult to follow the evolution of the full distribution function. Symmetry can greatly help, by reducing the number of free variables, which sometimes enables complete solutions that would not be possible without the symmetry. This theoretical argument is augmented by the practical fact that many astrophysical systems possess at least an approximate symmetry. The best way to analyze symmetric systems is to use matched coordinates that naturally take advantage of the symmetry of the system. In this chapter we will particularly be interested in systems with spherical symmetry, so we first use spherical coordinates to derive matching versions of the equations of stellar dynamics.

In spherical coordinates (R, θ, ϕ) , we use the corresponding unit vectors $\hat{R}, \hat{\theta}, \hat{\phi}$ to express the velocity of a particle in corresponding components:

$$\vec{v} = v_R \hat{R} + v_\theta \hat{\theta} + v_\phi \hat{\phi}, \quad (6.8)$$

where

$$v_R = \dot{R}, \quad v_\theta = R\dot{\theta}, \quad v_\phi = R\sin\theta\dot{\phi}. \quad (6.9)$$

Here $\dot{s}$ denotes ds/dt for any quantity s . Newton's Law for the acceleration of a particle, using the gradient in spherical coordinates, is

$$\frac{d\vec{v}}{dt} = -\vec{\nabla}\Phi = -\frac{\partial\Phi}{\partial R}\hat{R} - \frac{1}{R}\frac{\partial\Phi}{\partial\theta}\hat{\theta} - \frac{1}{R\sin\theta}\frac{\partial\Phi}{\partial\phi}\hat{\phi}. \quad (6.10)$$

On the left-hand side of this equation, the time derivative affects both the velocity components and the unit vectors in Eq. (6.8). The final result for the acceleration is (see Eq. 1B31 of [1]):

$$\begin{aligned} \frac{d\vec{v}}{dt} = & \left(\ddot{R} - R\dot{\theta}^2 - R\sin^2\theta\dot{\phi}^2 \right) \hat{R} + \left(2\dot{R}\dot{\theta} + R\ddot{\theta} - R\sin\theta\cos\theta\dot{\phi}^2 \right) \hat{\theta} \\ & + \left(R\sin\theta\ddot{\phi} + 2\dot{R}\sin\theta\dot{\phi} + 2R\cos\theta\dot{\phi}\dot{\theta} \right) \hat{\phi}. \end{aligned} \quad (6.11)$$

For example, the R -component of Newton's Law can be written as

$$\dot{v}_R = \ddot{R} = -\frac{\partial\Phi}{\partial R} + \frac{1}{R}(v_\theta^2 + v_\phi^2).$$

The physical meaning of this equation is that the radial velocity changes due to the radial gravitational force plus the (fictitious) centrifugal force. Or, if the tangential velocity terms are moved to the other side of the equation, then the equation says that the radial component of gravity must supply the centripetal force in order to keep R constant, and any remaining force causes the radius to change. The other components of the acceleration in Eq. (6.11) also show contributions of fictitious forces, namely the centrifugal force and the Coriolis force.

To derive the CBE in spherical coordinates, we substitute the spherical-coordinate expressions for the gradient and the acceleration in Eq. (6.5), and express the result in terms of the spherical coordinates and velocity components. The final result is (see Eq. 4.14 of [1]):

$$\begin{aligned} 0 = & \frac{\partial f}{\partial t} + v_R \frac{\partial f}{\partial R} + \frac{v_\theta}{R} \frac{\partial f}{\partial \theta} + \frac{v_\phi}{R\sin\theta} \frac{\partial f}{\partial \phi} + \left(\frac{v_\theta^2 + v_\phi^2}{R} - \frac{\partial\Phi}{\partial R} \right) \frac{\partial f}{\partial v_R} \\ & + \frac{1}{R} \left(v_\phi^2 \cot\theta - v_R v_\theta - \frac{\partial\Phi}{\partial \theta} \right) \frac{\partial f}{\partial v_\theta} \\ & - \frac{1}{R} \left[v_\phi(v_R + v_\theta \cot\theta) + \frac{1}{\sin\theta} \frac{\partial\Phi}{\partial \phi} \right] \frac{\partial f}{\partial v_\phi}. \end{aligned} \quad (6.12)$$

6.3. The spherical Jeans equation

In analogy with the derivation of the Euler equation in Cartesian coordinates, we wish to take the v_R moment $\int v_R d^3v$ of Eq. (6.12). We also assume a system that is in a *steady state* and that is *spherically symmetric*. The first assumption implies $\partial f / \partial t = 0$, and the second $\partial f / \partial \theta = \partial f / \partial \phi = 0$ as well as $\Phi = \Phi(R)$. Some additional implications of these assumptions will be pointed out as needed in the derivation that follows. We also note that while this is not necessary in what follows, the steady state assumption is often also assumed to imply no mean motion, i.e. $\overline{\vec{v}} = 0$, or at least no mean motion other than rotation about an axis (e.g. the z axis, so that only $\overline{v_\phi}$ may be non-zero).

With these assumptions, the first non-zero term in the v_R moment is

$$\int v_R d^3v \left(v_R \frac{\partial f}{\partial R} \right) = \frac{\partial}{\partial R} \left(n \overline{v_R^2} \right) = \frac{d}{dR} \left(n \overline{v_R^2} \right).$$

Here, in the first step we noted that the R derivative can be taken outside the velocity integral, and the resulting integral is simply the mean value of v_R^2 (except for the normalization factor n). In the second step we used the assumptions of a steady state and of spherical symmetry to note that any velocity-averaged quantity can only depend on R .

In the next non-zero term, the v_R integral is

$$\int v_R dv_R \frac{\partial f}{\partial v_R} = - \int f dv_R,$$

where integration by parts transferred the v_R derivative from f to v_R and added a minus sign; the integrated term vanished assuming that $f \rightarrow 0$ rapidly when $v_R \rightarrow \pm\infty$ (i.e. there are no particles with infinite kinetic energy). Note here that $d^3v = dv_R dv_\theta dv_\phi$, and the integral over velocity space is done at a fixed spatial position, and so (v_R, v_θ, v_ϕ) are simply velocity components in a three-dimensional coordinate system made up of three fixed, mutually-perpendicular directions. Thus, the contribution to the v_R moment from the $\partial f / \partial v_R$ term in Eq. (6.12) is

$$\frac{n}{R} \left(-\overline{v_\theta^2} - \overline{v_\phi^2} \right) + n \frac{d\Phi}{dR}.$$

For the remaining terms of the CBE, we similarly note that

$$\int v_\theta dv_\theta \frac{\partial f}{\partial v_\theta} = - \int f dv_\theta,$$

and similarly for v_ϕ . When the corresponding velocity component does not appear, we get,

$$\int dv_\theta \frac{\partial f}{\partial v_\theta} = 0,$$

again due to the boundary conditions of $f \rightarrow 0$ at high velocities. Thus, the final two f derivatives in Eq. (6.12) contribute this to the v_R moment:

$$\frac{n}{R} \overline{v_R^2} + \frac{n}{R} \left(\overline{v_R^2} + \overline{v_R v_\theta} \cot \theta \right).$$

We now also assume $\overline{v_R v_\theta} = 0$, which can be derived from various stronger assumptions, such as a distribution function that depends only on the magnitude (not the sign) of v_R or of v_θ . This is a kind of parity symmetry in the velocity-space dependence; for v_θ , in particular, this is a natural assumption, as we presently explain.

Collecting all the terms, we obtain

$$\frac{d}{dR} \left(n \overline{v_R^2} \right) + \frac{n}{R} \left[2\overline{v_R^2} - \left(\overline{v_\theta^2} + \overline{v_\phi^2} \right) \right] = -n \frac{d\Phi}{dR}. \quad (6.13)$$

To further simplify this equation, we assume that the velocity structure is invariant under rotation about the radial direction. Specifically, we assume that

$$\overline{v_\theta^2} = \overline{v_\phi^2}. \quad (6.14)$$

This assumes a symmetry of the velocity dispersion to a 90° rotation about the radial direction, from the $\hat{\theta}$ direction to $\hat{\phi}$. Note that the above parity symmetry for v_θ can be seen as a symmetry to a 180° rotation about the radial direction, from the $\hat{\theta}$ direction to $-\hat{\theta}$. An alternate assumption that yields these desired simplifications is that the distribution function depends on the radial and tangential components of the velocity (i.e. the components parallel to and perpendicular to $\vec{R}$, respectively), but not on the particular direction of the tangential component.

Next, we describe the relation between the radial and tangential components of the squared velocity dispersion using the anisotropy parameter

$$\beta \equiv 1 - \frac{\overline{v_\theta^2}}{\overline{v_R^2}}. \quad (6.15)$$

Note that an isotropic distribution corresponds to $\beta = 0$, while the case of purely radial orbits is $\beta = 1$. This finally yields what is often called the *spherical Jeans equation*:

$$\frac{1}{n} \frac{d}{dR} \left(n \overline{v_R^2} \right) + 2\beta \frac{\overline{v_R^2}}{R} = -\frac{d\Phi}{dR}. \quad (6.16)$$

An alternate form of the same equation can be derived by noting that the gravitational force, under the same assumption of spherical symmetry, is

$$-\frac{d\Phi}{dR} = -\frac{GM(R)}{R^2}, \quad (6.17)$$

where $M(R)$ is the enclosed mass within radius R . We thus obtain the mass distribution (expressed using the circular velocity):

$$v_c^2 = \frac{GM(R)}{R} = -\frac{\overline{v_R^2}}{2} \left(\frac{d \log n}{d \log R} + \frac{d \log \overline{v_R^2}}{d \log R} + 2\beta \right). \quad (6.18)$$

We have written this in terms of the logarithmic slopes of the distributions of density and of radial velocity dispersion. The important conclusion from this last equation is that if we can measure, for a stellar system, the following three distributions: $n(R)$, $\overline{v_R^2}$, and $\beta(R)$, then (under the above assumptions) we can infer the mass distribution $M(R)$. It is often possible to measure the projected intensity I and the projected line-of-sight velocity dispersion σ_P , each as a function of R . This still leaves one function unknown, so that a solution requires an additional assumption.

As a simple example, we assume $\beta = 0$, and then integrate along the line of sight at a projected distance h from the center of the spherical system (Fig. 6.1). We let R be the radial coordinate (i.e. the distance from the center) and z measure position along the line of sight, where $z = 0$ is the point of closest approach (where $R = h$). In general $h^2 + z^2 = R^2$, and so (for a fixed h) $zdz = RdR$. Then

$$I(h) = 2L_1 \int_{z=0}^{\infty} n \left(\sqrt{h^2 + z^2} \right) dz = 2L_1 \int_{R=h}^{\infty} \frac{n(R)RdR}{\sqrt{R^2 - h^2}}, \quad (6.19)$$

where L_1 is the (mean) luminosity of a star, so that $L_1 n$ is the stellar luminosity density. The factor of two accounts for the symmetric integration over negative z

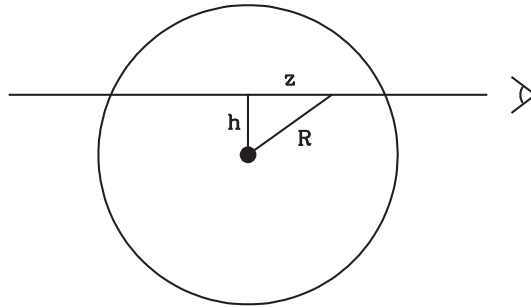


Fig. 6.1. Sketch for calculating the line-of-sight projection of a spherically symmetric distribution. Note that the line of sight, together with the center of the spherical distribution, determine a plane; the diagram is drawn in that plane.

values. The luminosity-weighted, projected, line-of-sight velocity dispersion $\sigma_P(h)$, which can be measured from spectral line widths, is similarly given by

$$I(h)\sigma_P^2(h) = 2L_1 \int_{R=h}^{\infty} \frac{n(R)\overline{v_R^2}(R) R dR}{\sqrt{R^2 - h^2}}, \quad (6.20)$$

where in the case of $\beta = 0$ the squared line-of-sight velocity dispersion is equal to $\overline{v_R^2}$. These two equations can be inverted using the Abel integral equation (see, e.g. Sec. B.5 of [1]), to find $L_1 n(R)$ and $L_1 n(R)\overline{v_R^2}(R)$; the first equation is solved as

$$n(R) = -\frac{1}{\pi L_1 R} \frac{d}{dR} \int_R^{\infty} dh \frac{h I(h)}{\sqrt{h^2 - R^2}}, \quad (6.21)$$

and the second one is similarly solved. At that point the mass profile can be found from Eq. (6.18), again under the assumption of $\beta = 0$.

6.4. The virial theorem

We have already used the virial theorem to derive an important result for non-linear spherical collapse in an Einstein–de Sitter Universe (Sec. 5.3). We present here a general proof of this theorem for steady-state, self-gravitating, collisionless systems.

We assume stars (or classical particles) with masses m_i , positions $\vec{x}_i$ and momenta $\vec{q}_i$, where the index i runs on all the stars. We first calculate:

$$\frac{d}{dt} \sum_i \vec{q}_i \cdot \vec{x}_i = \sum_i \frac{d\vec{q}_i}{dt} \cdot \vec{x}_i + \sum_i \vec{q}_i \cdot \frac{d\vec{x}_i}{dt} = - \sum_i m_i \vec{\nabla} \Phi(\vec{x}_i) \cdot \vec{x}_i + \sum_i m_i v_i^2.$$

In a steady state, the above time derivative is zero, so we obtain

$$\frac{1}{2} \sum_i m_i \vec{x}_i \cdot \vec{\nabla} \Phi = \frac{1}{2} \sum_i m_i v_i^2. \quad (6.22)$$

Transforming now to the continuous case, $\sum_i$ becomes a volume integral over position $\vec{x}$, where at each $\vec{x}$ the sum of m_i over stars at that position is replaced by ρd^3x in terms of the volume density ρ , and the sum of $m_i v_i^2$ becomes $\rho \overline{v^2} d^3x$, where $\overline{v^2}$ is the mass-weighted average of v^2 for stars at position $\vec{x}$. Thus,

$$\frac{1}{2} \int \rho \vec{x} \cdot \vec{\nabla} \Phi d^3x = \frac{1}{2} \int \rho \overline{v^2} d^3x. \quad (6.23)$$

The right-hand side is the total kinetic energy, K . We want to show that the left-hand side is related to the total potential energy. We will call the left-hand side $(-W/2)$, and explore the quantity W .

The Newtonian potential is given by

$$\Phi(\vec{x}) = -G \int \frac{\rho(\vec{y})}{|\vec{x} - \vec{y}|} d^3y. \quad (6.24)$$

Noting that

$$\vec{\nabla} \frac{1}{r} = -\frac{\vec{r}}{r^3}, \quad (6.25)$$

we can re-write W as

$$W = G \int \int \rho(\vec{x}) \rho(\vec{y}) \vec{x} \cdot \frac{\vec{y} - \vec{x}}{|\vec{y} - \vec{x}|^3} d^3x d^3y.$$

This expression remains unchanged if we switch the labels $\vec{x}$ and $\vec{y}$. This switch changes $\vec{x} \cdot (\vec{y} - \vec{x})$ to $\vec{y} \cdot (\vec{x} - \vec{y})$. We get the same result if we take the mean of the two expressions (the original and the switched one). In this mean we have the term

$$\frac{1}{2} [\vec{x} \cdot (\vec{y} - \vec{x}) + \vec{y} \cdot (\vec{x} - \vec{y})] = \frac{1}{2} (\vec{x} - \vec{y}) \cdot (\vec{y} - \vec{x}) = -\frac{1}{2} |\vec{x} - \vec{y}|^2.$$

Thus, we find

$$W = -\frac{1}{2} G \int \int \rho(\vec{x}) \rho(\vec{y}) \frac{1}{|\vec{y} - \vec{x}|} d^3x d^3y = \frac{1}{2} \int \rho(\vec{x}) \Phi(\vec{x}) d^3x. \quad (6.26)$$

We now find the total potential energy, U , of the system. It can be calculated as the sum of changes in the potential energy due to gravity as we assemble the system, $\delta\rho$ at a time. At each step, given the current gravitational potential field $\Phi(\vec{x})$, the change in the potential energy due to adding $\delta\rho(\vec{x})$ is

$$\delta U = \int \delta\rho(\vec{x}) \Phi(\vec{x}) d^3x. \quad (6.27)$$

This is negative, since gravity naturally attracts $\delta\rho$ from infinity. We now use the Poisson equation to see that

$$\nabla^2 \Phi = 4\pi G \rho; \quad \nabla^2 \delta\Phi = 4\pi G \delta\rho.$$

Thus, the changes in this step of the potential energy and of the gravitational potential are related through

$$\delta U = \frac{1}{4\pi G} \int \nabla^2(\delta\Phi) \Phi d^3x. \quad (6.28)$$

We now use the vector calculus relation (based on the product rule of differentiation):

$$\vec{\nabla} \cdot (\Phi \vec{\nabla} \delta\Phi) = \Phi \nabla^2(\delta\Phi) + \vec{\nabla} \Phi \cdot \vec{\nabla}(\delta\Phi)$$

to do essentially an integration by parts, getting

$$\delta U = -\frac{1}{4\pi G} \int \vec{\nabla} \Phi \cdot \vec{\nabla}(\delta\Phi) d^3x. \quad (6.29)$$

Here we dropped the “integrated term”, which was the volume integral of a divergence, which by the divergence theorem is equal to an integral over the surface area of the boundary (at infinity), where we assume that Φ and $\delta\Phi$ both vanish. The next step is similar: we use the vector calculus relation

$$\vec{\nabla} \cdot (\delta\Phi \vec{\nabla}\Phi) = \delta\Phi \nabla^2\Phi + \vec{\nabla}(\delta\Phi) \cdot \vec{\nabla}\Phi$$

to do a similar integration by parts, again dropping the integrated term at infinity, thus obtaining

$$\delta U = \frac{1}{4\pi G} \int \delta\Phi \nabla^2\Phi d^3x = \int (\delta\Phi)\rho d^3x. \quad (6.30)$$

Overall, we have performed two integrations by part, in order to transfer the Laplacian from $\delta\Phi$ to Φ . We now have two expressions for δU , from Eq. (6.27) and Eq. (6.30). They are equal, and thus both also equal their mean:

$$\delta U = \frac{1}{2} \int [\delta\rho \Phi + (\delta\Phi)\rho] d^3x = \frac{1}{2} \int \delta(\rho\Phi) d^3x, \quad (6.31)$$

where the final integral is over the change, in this step, of the product $\rho\Phi$. Adding up all these small changes yields the total:

$$U = \frac{1}{2} \int \rho\Phi d^3x = W, \quad (6.32)$$

where in the last step we noted Eq. (6.26). Then Eq. (6.23) finally becomes $-U/2 = K$, which is the virial theorem:

$$E = U + K = \frac{U}{2} = -K. \quad (6.33)$$

We have only assumed a steady-state system moving under its own gravity. Note that one consequence is that the total energy $E < 0$, i.e. the system is gravitationally bound.

A particularly simple example of a virialized system is an object of mass m in a circular orbit about a mass M . In this case,

$$\frac{v^2}{R} = \frac{GM}{R^2},$$

and

$$U = -\frac{GMm}{R}; \quad K = \frac{1}{2}mv^2 = -\frac{1}{2}U.$$

6.5. Constants and integrals of motion

In this section we go back to the CBE, and discuss some general classes of solutions. First we define two important concepts. A constant of motion $C(\vec{x}, \vec{v}, t)$ and an integral of motion $I(\vec{x}, \vec{v})$ are both unchanged along a trajectory:

$$\frac{d}{dt}I(\vec{x}, \vec{v}) = 0 ; \quad \frac{d}{dt}C(\vec{x}, \vec{v}, t) = 0. \quad (6.34)$$

Recalling that the CBE can be written simply as $df/dt = 0$, we see that a class of solutions can be built on integrals of motion:

$$\frac{d}{dt}f[I_1(\vec{x}, \vec{v}), \dots, I_n(\vec{x}, \vec{v})] = \sum_{m=1}^n \frac{\partial f}{\partial I_m} \frac{dI_m}{dt} = 0. \quad (6.35)$$

Thus, any f of this form is automatically a solution of the CBE. Here integrals of motion are commonly used rather than constants of motion, in order to find steady-state solutions (without an explicit time dependence).

Two important examples of integrals of motion are the energy and the angular momentum. The energy (per unit mass) is

$$E = \frac{1}{2}v^2 + \Phi(\vec{R}, t), \quad (6.36)$$

where we use $\vec{R}$ for position. In general,

$$\frac{dE}{dt} = \vec{v} \cdot \frac{d\vec{v}}{dt} + \frac{d\Phi}{dt} = -\vec{v} \cdot \vec{\nabla}\Phi + \left(\frac{\partial\Phi}{\partial t} + \vec{v} \cdot \vec{\nabla}\Phi \right) = \frac{\partial\Phi}{\partial t}. \quad (6.37)$$

Thus, in a steady state (when Φ is not a function of time), the energy is constant along a trajectory; in this case, also, the energy is an integral of motion (and not just a constant of motion). Note that a form of energy conservation can also sometimes be valid in evolving cases, such as the spherical collapse problem that we considered in Sec. 5.1.

The angular momentum (per unit mass) is

$$\vec{L} = \vec{R} \times \vec{v}, \quad (6.38)$$

and it evolves according to

$$\frac{d\vec{L}}{dt} = \vec{v} \times \vec{v} + \vec{R} \times \frac{d\vec{v}}{dt} = -\vec{R} \times \vec{\nabla}\Phi, \quad (6.39)$$

where we used the fact that any vector crossed with itself gives zero. Thus, in any spherical potential $\Phi(R, t)$, $\vec{\nabla}\Phi$ is in the radial direction and the three components of $\vec{L}$ are integrals of motion.

If we can assume both steady-state and spherical conditions, we can solve the CBE with $f = f(E, \vec{L})$. If we add further symmetry, we can try the simpler $f = f(E, L)$.

6.6. The isothermal sphere

A simple but important example of a steady-state solution with spherical symmetry is an isothermal sphere. This example is particularly simple as it has no L dependence. Let

$$f = f(E) = \frac{\rho_1}{(2\pi\sigma^2)^{3/2}} e^{(-\Phi - \frac{1}{2}v^2)/\sigma^2}, \quad (6.40)$$

which includes two fixed parameters (σ and ρ_1); note that we use f here to refer to the mass (not number) density. Then the corresponding mass distribution is

$$\rho = \int f d^3v = \rho_1 e^{-\Phi/\sigma^2}, \quad (6.41)$$

since the integral over each component of velocity gives a Gaussian normalization factor of $\sigma \sqrt{2\pi}$. We demand consistency with the other relation between ρ and Φ , namely the Poisson equation:

$$4\pi G\rho = \nabla^2\Phi = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\Phi}{dr} \right), \quad (6.42)$$

where r is the spherical radial coordinate. Combining these two equations yields an equation for ρ :

$$\frac{d}{dr} \left(r^2 \frac{d \log \rho}{dr} \right) = -\frac{4\pi G}{\sigma^2} r^2 \rho. \quad (6.43)$$

6.6.1. Isothermal gas analogy

Consider a static, spherically-symmetric ideal gas in hydrostatic equilibrium, i.e. where its pressure gradient balances its self-gravity. Then

$$\frac{1}{\rho} \frac{dp}{dr} = \frac{1}{\rho} \frac{k_B T}{\mu} \frac{d\rho}{dr} = -\frac{GM(r)}{r^2}, \quad (6.44)$$

where in the first step we assumed the gas is isothermal at a fixed temperature T . We multiply this equation by $r^2 \mu / k_B T$ to obtain

$$\frac{r^2}{\rho} \frac{d\rho}{dr} = -\frac{\mu}{k_B T} GM(r). \quad (6.45)$$

Next, we take a radial derivative:

$$\frac{d}{dr} \left(r^2 \frac{d \log \rho}{dr} \right) = -\frac{G\mu}{k_B T} 4\pi r^2 \rho. \quad (6.46)$$

This is mathematically identical to Eq. (6.43) through the correspondence

$$\sigma^2 \longleftrightarrow \frac{k_B T}{\mu}.$$

This is why the example at the beginning of this section is called an isothermal sphere, even though it may correspond to a system of collisionless stars or dark matter particles.

Another part of the analogy can be seen in the velocity distribution. The distribution function of Eq. (6.40) is exponential in v^2 , which corresponds to the Maxwell-Boltzmann distribution of velocities in an ideal gas. We can see the meaning of σ by noting that

$$\overline{v^2} = \frac{\int v^2 e^{-\frac{1}{2}\frac{v^2}{\sigma^2}} d^3v}{\int e^{-\frac{1}{2}\frac{v^2}{\sigma^2}} d^3v} = 3\sigma^2.$$

By symmetry, we then have

$$\overline{v_x^2} = \overline{v_y^2} = \overline{v_z^2} = \sigma^2.$$

Thus, σ is the one-dimensional velocity dispersion (in any direction).

6.6.2. The singular isothermal sphere (SIS)

In general, the solution to Eq. (6.43) is a bit complicated. A particularly simple analytical solution is given by a power law. If we assume

$$\rho = Cr^{-b},$$

then substituting this into Eq. (6.43) yields

$$-b = -\frac{4\pi G}{\sigma^2} Cr^{2-b}.$$

Thus, the solution requires $b = 2$, which yields the constant C and the solution:

$$\rho(r) = \frac{\sigma^2}{2\pi Gr^2}, \quad (6.47)$$

which corresponds to

$$M(r) = \int 4\pi r^2 \rho dr = \frac{2\sigma^2}{G} r. \quad (6.48)$$

The circular velocity is

$$V_c = \sqrt{\frac{GM(r)}{r}} = \sqrt{2}\sigma, \quad (6.49)$$

i.e. constant with radius. Thus, the singular isothermal sphere is a rough first model for galactic halos (which are dominated by dark matter), as it corresponds to the

observed flat rotation curves. The corresponding potential is

$$\Phi = 2\sigma^2 \ln r + \tilde{C}, \quad (6.50)$$

where $\tilde{C}$ is a constant. This power-law solution of ρ is singular at the origin, hence is known as a singular isothermal sphere (SIS). This model is particularly commonly used in gravitational lensing (Chap. 8). For that we will need the projected surface mass density, at a projected radius R (see Fig. 6.1):

$$\Sigma(R) = 2 \int_{r=R}^{\infty} \rho(r) \frac{r dr}{\sqrt{r^2 - R^2}} = \frac{\sigma^2}{2GR}. \quad (6.51)$$

Reference

- [1] J. Binney, S. Tremaine, *Galactic Dynamics*: Second Edition, by James Binney and Scott Tremaine. ISBN 978-0-691-13026-2 (HB). Published by Princeton University Press, Princeton, NJ USA, 2008.

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Chapter 7

Galactic Disks and Spiral Structure

In this chapter we look within galaxies and try to decipher their most spectacular observed property, namely, the spiral arms of disk galaxies. We follow [1] in presenting the explanation of spiral structure due to Lin & Shu [2].

7.1. Cylindrical coordinates and disks

Galactic disks possess approximate azimuthal symmetry. To take advantage of this symmetry, it is advantageous to work in cylindrical coordinates. Denoting the coordinates (R, ϕ, z) , the velocity in cylindrical components is

$$\vec{v} = \dot{R}\hat{R} + R\dot{\phi}\hat{\phi} + \dot{z}\hat{z}, \quad (7.1)$$

and the acceleration is (Eq. B24 of [1])

$$\frac{d\vec{v}}{dt} = \left(\ddot{R} - R\dot{\phi}^2\right)\hat{R} + (2\dot{R}\dot{\phi} + R\ddot{\phi})\hat{\phi} + \ddot{z}\hat{z}. \quad (7.2)$$

The equation of motion (Newton's Law) is

$$\frac{d\vec{v}}{dt} = -\vec{\nabla}\Phi = -\frac{\partial\Phi}{\partial R}\hat{R} - \frac{1}{R}\frac{\partial\Phi}{\partial\phi}\hat{\phi} - \frac{\partial\Phi}{\partial z}\hat{z}. \quad (7.3)$$

We assume an axisymmetric potential, $\Phi = \Phi(R, z)$, which moreover is symmetric about $z = 0$ (as disk galaxies appear to be, to a good approximation):

$$\Phi(R, z) = \Phi(R, -z). \quad (7.4)$$

The z -component of angular momentum (per unit mass) is particularly useful in cylindrical coordinates:

$$L_z = \hat{z} \cdot \vec{L} = \hat{z} \cdot (\vec{r} \times \vec{v}) = \vec{v} \cdot (\hat{z} \times \vec{r}) = Rv_\phi = R^2\dot{\phi}, \quad (7.5)$$

where we used the cyclic shift property of the scalar triple product, and then the fact that $\hat{z} \times \vec{r} = R\hat{\phi}$. We now see that

$$\frac{dL_z}{dt} = 2R\dot{R}\dot{\phi} + R^2\ddot{\phi} = R(2\dot{R}\dot{\phi} + R\ddot{\phi}). \quad (7.6)$$

The equation of motion thus yields the following three equations (for an axisymmetric potential):

$$\ddot{R} - R\dot{\phi}^2 = -\frac{\partial\Phi}{\partial R}; \quad \ddot{z} = -\frac{\partial\Phi}{\partial z}; \quad R^2\dot{\phi} = L_z = \text{const.} \quad (7.7)$$

The last equation, which arose from the ϕ component, expresses the conservation of L_z , and is equivalent to Kepler's Second Law (the Law of Equal Areas).

We can alternatively write the first two equations in the form of Newton's Law in two Cartesian coordinates:

$$\ddot{R} = -\frac{\partial\Phi_{\text{eff}}}{\partial R}; \quad \ddot{z} = -\frac{\partial\Phi_{\text{eff}}}{\partial z}, \quad (7.8)$$

where

$$\Phi_{\text{eff}} \equiv \Phi(R, z) + \frac{L_z^2}{2R^2}. \quad (7.9)$$

We note that the angular momentum part of the effective potential acts as an angular momentum barrier which prevents the star from reaching very low R , for a given L_z and energy. Most importantly, we see that a circular orbit (i.e. fixed R) at a fixed z requires

$$\vec{\nabla}\Phi_{\text{eff}} = 0, \quad (7.10)$$

where this is a two-dimensional gradient [treating (R, z) as two dimensions equivalent to the normal (x, y)]. In addition, symmetry about $z = 0$ allows us to derive an additional result, as follows. We first note that (denoting $\partial\Phi/\partial z$ as $\partial_z\Phi$)

$$\partial_z\Phi(z) = \partial_z[\Phi(-z)] = -(\partial_z\Phi)|_{-z}.$$

Substituting $z = 0$ into this yields, as a general result,

$$0 = \left. \frac{\partial\Phi}{\partial z} \right|_{z=0} = \left. \frac{\partial\Phi_{\text{eff}}}{\partial z} \right|_{z=0}. \quad (7.11)$$

Thus, for a circular orbit at $z = 0$, Eq. (7.10) really implies only one condition:

$$\left. \frac{\partial\Phi}{\partial R} \right|_{(R_g, z=0)} = \frac{L_z^2}{R_g^3} = R_g\dot{\phi}^2. \quad (7.12)$$

The last step shows that this condition is simply the requirement that gravity provide the needed centripetal acceleration. In this equation we have used the notation R_g , which henceforth automatically refers to a circular orbit in the plane; below, we use such orbits as a reference ("guiding center") for more complicated orbits.

7.2. Theory of epicycles

Circular orbits in a plane are too simple for even an approximate analysis of galactic disks. For a more realistic description that is nonetheless analytically tractable, nearly-circular orbits are used, and analyzed as small perturbations with respect to planar circular orbits.

We first note that the energy (per unit mass) can be written as

$$E = \frac{1}{2}v^2 + \Phi = \frac{1}{2} \left(\dot{R}^2 + \dot{z}^2 \right) + \Phi_{\text{eff}}.$$

In particular, for orbits in the plane ($z = 0$),

$$E = \frac{1}{2} \left[\dot{R}^2 + \frac{L_z^2}{R^2} \right] + \Phi(R, 0).$$

This shows that, for a given L_z , among planar orbits that pass through R , the circular orbit is the one with minimum E .

As in the previous section, for a given perturbed orbit we refer to the reference circular orbit as having radius R_g (as well as energy E_g , etc.), where this guiding center is defined (for the same value of L_z as the perturbed orbit) by Eq. (7.10), which as we saw implies Eq. (7.12); the latter equation usually has a single solution R_g for each value of L_z . The perturbed orbit must then have a slightly higher energy E , with $E - E_g \ll |E_g|$. Let the perturbed radial position be

$$x \equiv R - R_g. \quad (7.13)$$

Then we can write

$$\Phi_{\text{eff}} \simeq C + \frac{1}{2}(\kappa^2 x^2 + \nu^2 z^2), \quad (7.14)$$

since we saw in the last section that $\vec{\nabla}\Phi_{\text{eff}} = 0$ for the circular orbit (so there are no first-order terms in this Taylor expansion of Φ_{eff} with respect to the circular orbit), and we also saw [Eq. (7.11)] that $\partial\Phi_{\text{eff}}/\partial z = 0$ anywhere in the plane (including when $z = 0$ but x is non-zero; so there is no xz term). The coefficients of this expansion are

$$\kappa^2 \equiv \left. \frac{\partial^2 \Phi_{\text{eff}}}{\partial R^2} \right|_{(R_g, 0)} = \left. \frac{\partial^2 \Phi}{\partial R^2} \right|_{(R_g, 0)} + \frac{3L_z^2}{R_g^4}, \quad (7.15)$$

and

$$\nu^2 \equiv \left. \frac{\partial^2 \Phi}{\partial z^2} \right|_{(R_g, 0)}. \quad (7.16)$$

We use Ω to denote the angular frequency of the circular orbit:

$$\Omega^2(R) = \left(\frac{v_{\text{circ}}}{R} \right)^2 = \dot{\phi}_g^2 = \frac{L_z^2}{R^4} = \frac{1}{R} \left. \frac{\partial \Phi}{\partial R} \right|_{(R_g, 0)}, \quad (7.17)$$

where the last step used Eq. (7.12). We now see that

$$\frac{d}{dR}\Omega^2 = \frac{1}{R} \frac{\partial^2 \Phi}{\partial R^2} \Big|_{(R_g, 0)} - \frac{1}{R}\Omega^2. \quad (7.18)$$

Together with Eq. (7.15), this gives an important relation between Ω and κ :

$$\kappa^2 = R \frac{d\Omega^2}{dR} + 4\Omega^2. \quad (7.19)$$

The *equations of motion* [Eq. (7.8)] can now be written in the form

$$\ddot{x} = -\frac{\partial \Phi_{\text{eff}}}{\partial x} \simeq -\kappa^2 x ; \quad \ddot{z} \simeq -\nu^2 z. \quad (7.20)$$

The solution to each equation is an oscillatory function of time, with two free parameters (an amplitude and phase):

$$x(t) = X \cos(\kappa t + \Psi_x) ; \quad z(t) = Z \cos(\nu t + \Psi_z). \quad (7.21)$$

κ is called the “epicyclic frequency”; it is the frequency of the radial oscillations of nearly-circular orbits about the circular guiding center. We are less interested in the z motion (which is in any case independent, given our approximations) and more in planar orbits.

Since the circular plus epicyclic motion determines the shape of planar orbits, it is of interest to consider the relation [Eq. (7.19)] between the circular angular frequency and the epicyclic frequency in particular examples. For motion around a **point mass** M ,

$$\Omega^2 = \frac{V_c^2}{R^2} = \frac{1}{R} \frac{GM}{R^2} = \frac{GM}{R^3}.$$

We note that Ω depends on R , which is termed *differential rotation*. We see that $\kappa^2 = \Omega^2[-3 + 4]$ so that $\kappa = \Omega$. This implies perfect synchronization between the epicycle and the guiding star, which implies a closed orbit: indeed, it is an ellipse in this case. The case of **solid body rotation** (or such motion, even if there is no actual solid body) is constant Ω with radius. This yields $\kappa = 2\Omega$. A **flat rotation curve** (corresponding to the SIS of Sec. 6.6.2) has $\Omega^2 = V_c^2/R^2$ with a constant circular velocity V_c . Thus, $\kappa = \sqrt{2}\Omega$ in this case. Finally, for the Sun (in its motion around the Galactic center), current measurements of stellar proper motions with the Gaia satellite [3] imply $\kappa/\Omega = 1.32 \pm 0.02$. We note that when the ratio κ/Ω is rational, this implies a closed orbit (since after some finite number of complete circular orbits, the epicycle also has completed a finite number of its periods, and the entire motion then repeats). In particular, if this ratio is equal to the ratio between two small integers, then the orbital shape is relatively simple. At the other extreme, an irrational ratio implies an orbit that never closes.

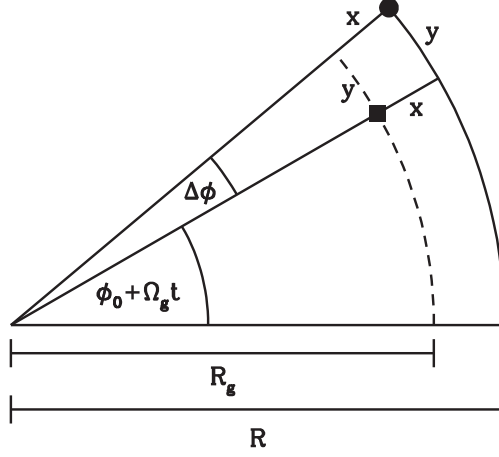


Fig. 7.1. Schematic drawing showing basic definitions of epicyclic motion in the plane. The orbital position (●) is described in terms of radial component x and azimuthal component y , each measured with respect to the guiding center (■). Note that the two arcs of length marked y are equal to first order (one of them is length $R_g \Delta\phi$ and the other $R \Delta\phi$).

We have not thus far examined the azimuthal motion. It does not need to be solved separately, as it is determined by the conservation of the z -component of the angular momentum:

$$\dot{\phi} = \frac{L_z}{R^2} = \frac{L_z}{R_g^2} \left(1 + \frac{x}{R_g}\right)^{-2} \simeq \Omega_g \left(1 - \frac{2x}{R_g}\right).$$

Given the solution for $x(t)$ in Eq. (7.21), we obtain

$$\phi = \phi_0 + \Omega_g t - \frac{2\Omega_g X}{\kappa R_g} \sin(\kappa t + \Psi_x). \quad (7.22)$$

We now measure the azimuthal position with respect to the circular motion of the guiding center (see Fig. 7.1):

$$y \equiv R[\phi - (\phi_0 + \Omega_g t)] \simeq -\frac{2\Omega_g}{\kappa} X \sin(\kappa t + \Psi_x), \quad (7.23)$$

where we multiplied by R in order to get arc-length.

Combining this with Eq. (7.21) shows that the shape of the epicycle is an ellipse in (x, y) :

$$x^2 + \left(\frac{\kappa y}{2\Omega_g}\right)^2 = X^2. \quad (7.24)$$

Thus, x varies in the range $-X \rightarrow X$, and y ranges over the same times ($2\Omega_g/\kappa$). The periods of the circular and epicyclic motion, respectively, are $T_g = 2\pi/\Omega_g$ and $T_{\text{epi}} = 2\pi/\kappa$. Historically, epicycles were key elements of pre-Copernican astronomical systems; however, Hipparchus and Ptolemy assumed circular epicycles, which

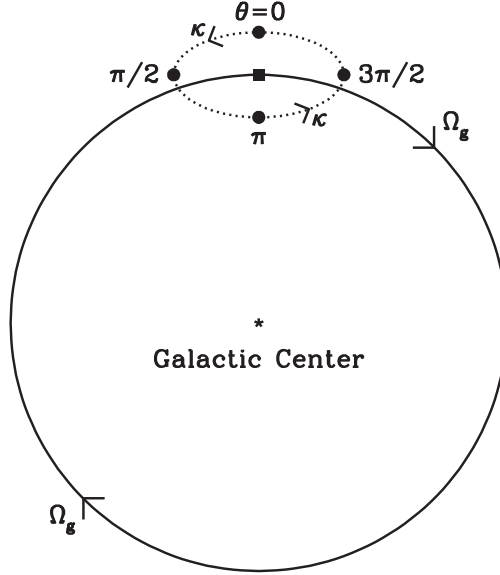


Fig. 7.2. Schematic drawing showing the rotation direction of an epicycle for a stellar orbit in a galactic disk. In this example, the guiding star (■) rotates clockwise around the Galactic Center, at an angular frequency Ω_g . The epicyclic motion (elliptic in this illustration, corresponding to the Keplerian problem) is counter-clockwise at an angular frequency κ , with the positions (●) shown at several values of the epicyclic phase θ .

would be correct for solid body rotation, but not for the Keplerian problem of rotation around a point mass (namely the Sun).

Denoting the phase as $\theta \equiv \kappa t + \Psi_x$, we can see that the fact that x goes as $\cos \theta$ and y as $-\sin \theta$ corresponds to retrograde motion; i.e. the epicyclic rotation is opposite to the rotation direction of the circular motion (see Fig. 7.2). Retrograde orbits are a direct consequence of the conservation of the z component of the angular momentum. This conservation (the Law of Equal Areas) requires smaller $\dot{\phi}$ at larger R ; since $\dot{\phi}$ is the sum of the constant guiding center motion plus the epicycle, the epicyclic rotation must be opposite to the guide rotation when $R > R_g$ (Recall that the guiding center is defined as having the same value of L_z , but at a constant R_g).

7.2.1. Oort constants

The Galactic rotation of stars near the Sun in the Milky Way disk is traditionally described in terms of the *Oort constants*, defined as

$$A = -\frac{1}{2}R\frac{d\Omega}{dR} ; \quad B = -\left(\frac{1}{2}R\frac{d\Omega}{dR} + \Omega\right). \quad (7.25)$$

Thus,

$$\Omega = A - B ; \quad \kappa^2 = -4B\Omega. \quad (7.26)$$

The value of A can be determined by measuring differential rotation. Then, B can be determined from the root-mean-square velocities in the x and y directions (defined relative to the guiding center, as above):

$$\frac{\langle v_y^2 \rangle^{1/2}}{\langle v_x^2 \rangle^{1/2}} = \frac{2\Omega}{\kappa}. \quad (7.27)$$

See Sec. 3.2.3 of [1] for a derivation of this and for more details. Current measurements with the Gaia satellite [3] give

$$A = 15.3 \pm 0.4 \text{ km s}^{-1} \text{ kpc}^{-1} ; \quad B = -11.9 \pm 0.4 \text{ km s}^{-1} \text{ kpc}^{-1}. \quad (7.28)$$

7.3. Spiral structure: derivation

7.3.1. The winding problem

In the quest to understand the spectacular spiral structure of disk galaxies, an important hurdle to be overcome is known as the *winding problem*. The issue is as follows.

Assume a differentially rotating disk. Suppose we follow a small portion at radius R of a spiral arm, whose direction is described by a *Pitch angle* i measured with respect to the azimuthal direction. If we measure position along the arm as $\phi(R)$, then

$$\cot i = \left| \frac{R d\phi}{dR} \right|. \quad (7.29)$$

The positions of stars (neglecting epicycles for this rough argument) change as

$$\phi(R, t) = \phi_0(R) + \Omega(R)t,$$

where $\phi_0(R)$ is the spiral arm shape at an initial time $t = 0$. Under differential rotation, and assuming that the spiral arm is marked by fixed, orbiting, stars, this should cause the pitch angle to change by

$$\Delta \cot i \sim \left| R t \frac{d\Omega(R)}{dR} \right| \sim t \frac{V_c}{R},$$

where in the last step we assumed that $d\Omega/dR$ is of order Ω/R , and used the circular (i.e. rotational) velocity V_c . The expected number of solar Galactic orbits over the $\sim 10^{10}$ yr lifetime of the Milky Way is

$$\frac{t}{2\pi R/V_c} \sim \frac{10^{10} \text{ yr}}{2\pi(8 \text{ kpc})/200 \text{ km/s}} \sim 40.$$

Thus, we expect $\cot i \sim 2\pi \times 40 \sim 250$, or an angle $i \sim 1/250 \sim 0.2^\circ$. Real spiral arms are not observed to be so tightly wound, with such small pitch angles. In the Milky Way and similar large spirals, a typical value is $i \sim 15^\circ$. Thus, the assumption made in this argument, that spiral arms correspond to fixed stars over time, must

be false. Instead, spiral arms must be density patterns, where the material within the arms changes over time.

7.3.2. *Spiral density waves*

In the remainder of this section we construct the accepted theory of the basic explanation of spiral structure [2]. The explanation is only approximate, and a detailed discussion of its limitations and extensions can be found in Chap. 6 of [1].

The basic idea is to describe the spiral structure as a stationary density wave, which is a perturbation to the underlying galactic disk. The logical structure of the derivation is as follows. Assuming a spiral density wave implies a perturbed gravitational potential (through the Poisson equation). This in turn perturbs the stellar orbits (which are determined by motion under gravity). Finally, for consistency we must close the loop: The resulting stellar orbits must give a stellar density that exactly corresponds to the density wave originally assumed.

7.3.3. *Equation of a spiral arm*

We begin by describing a spiral structure. As before, the position (e.g. of the peak density of a spiral arm) can be written as $\phi(R, t)$, but we now write

$$\phi(R, t) = g(R, t) + \frac{2\pi}{m}l, \quad (7.30)$$

where $l = 0, \dots, m-1$ describes m identical arms (one for each value of l). An alternate form is to multiply by m and write

$$m\phi + f(R, t) = 2\pi l, \quad (7.31)$$

where $f(R, t)$ is called the *shape function*. From this expression we see that the radial distance ΔR between adjacent arms at a given ϕ is

$$|f(R + \Delta R, t) - f(R, t)| = 2\pi. \quad (7.32)$$

7.3.4. *Tight-winding approximation*

In order to make the solution analytically tractable, it is helpful to assume the *tight winding* approximation, under which the spiral pattern is tightly wound, meaning that the various arms of the spiral structure are wound close together, and Eq. (7.32) can be written as

$$\left| \frac{\partial f}{\partial R} \right| \Delta R = 2\pi, \quad (7.33)$$

where $\Delta R \ll R$. The distance between consecutive spiral-arm peaks defines the radial wavelength of the spiral pattern:

$$\lambda(R, t) \equiv \frac{2\pi}{|\partial f(R, t)/\partial R|}, \quad (7.34)$$

which corresponds to a radial wavenumber

$$k(R, t) \equiv \frac{\partial f}{\partial R}. \quad (7.35)$$

Note that the pitch angle of a spiral arm is given by

$$\cot i = |R \partial \phi / \partial R| = |(R/m) \partial f / \partial R| = |kR/m|.$$

Thus, the condition needed for the tight-winding approximation is

$$1 \ll \frac{R}{\Delta R} = \frac{R}{2\pi/|k|} = \frac{m}{2\pi} \cot i.$$

In real spiral galaxies, $i \sim 15^\circ$, so $\cot i \sim 4$, and m is a few. Thus, the tight-winding approximation is only marginally valid (it does a bit better in the form $kR \gg 1$ which we will mostly need to assume); more complex analytical or numerical approaches are required for realistic predictions. However, we will make this approximation as it leads to an analytical result that yields great physical insight.

7.3.5. Surface density

The first step in building a spiral density wave is to construct the desired density structure. We assume that the surface density of the disk is

$$\Sigma = \Sigma_0(R) + \Sigma_1(R, \phi, t), \quad (7.36)$$

where Σ_1 is a perturbation of Σ_0 . In order to obtain a simple analytical solution, we will only keep terms to linear order in the perturbation. We want Σ_1 to have a spiral pattern:

$$\Sigma_1 = H(R, t) e^{i[m\phi + f(R, t)]}. \quad (7.37)$$

Here, H is the smooth form of the density along a given spiral arm, while the exponential contains the desired structure of multiple arms. This is a wave solution (similar in spirit to a Fourier decomposition), which uses a complex exponential (so that the physical Σ_1 is the real part). Note that the ϕ portion of such a wave solution must have an exponent of the form $im\phi$ with integer m , for consistency with having a well-defined value at a given position (which is unchanged when ϕ increases by 2π). Thus, the periodic nature of the angle ϕ automatically produces discreteness in the possible ϕ coefficients (which are basically the angular wavenumbers), and this helps explain the simple, spectacular symmetry of spiral arms.

Now, under the tight-winding approximation, Σ_1 undergoes many oscillations versus R (at a given ϕ). Distant oscillations will cancel out in their contribution to the potential Φ , implying that the perturbed potential at a given point is **local**, i.e. determined locally by nearby radii only. This means that we can make a local

(first-order) approximation of the shape function (near some radius R_0) based on the previous subsection:

$$f(R, t) \simeq f(R_0, t) + k(R_0, t)(R - R_0). \quad (7.38)$$

Now, under the tight-winding approximation, the variation of f with R (going from one spiral arm to the next) is rapid, while in comparison, H varies slowly with R (the density varies smoothly along an arm, or between adjacent arms at the same phase), and Σ varies slowly with ϕ (since i is small, the radial distance ΔR between consecutive arms is much smaller than the tangential arc-length between arms, $2\pi R/m$). Thus, our local approximation for the surface density is

$$\Sigma_1 = \Sigma_a e^{ik(R_0, t)(R - R_0)}, \quad (7.39)$$

where

$$\Sigma_a = H(R_0, t) e^{i[m\phi_0 + f(R_0, t)]}. \quad (7.40)$$

This corresponds to a plane wave with $\vec{k} = k\hat{R}$ (the direction $\hat{R}$ is essentially constant within a distance ΔR of $\vec{R}$).

7.3.6. Plane-wave potential

Now that we have established a plane wave form for the density perturbation, the next step is to solve for the resulting potential perturbation. We use Cartesian coordinates, and assume a plane-wave density perturbation in the x direction. We assume a thin disk, i.e. that the density is concentrated within an infinitesimal length in z (specifically, much smaller than the wavelength of the plane wave). The Poisson equation is

$$(\partial_x^2 + \partial_y^2 + \partial_z^2)\Phi = 4\pi G\rho = 4\pi G\Sigma_a e^{ikx} \delta_D(z). \quad (7.41)$$

We guess the form of the solution:

$$\Phi = \Phi_a e^{ikx - |kz|}.$$

It is trivial to see that this satisfies the Poisson equation at $z \neq 0$, since it gives $\nabla^2 \Phi = 0$. The non-trivial part is the boundary condition at $z = 0$. To calculate it, we apply $\int_{-\epsilon}^{\epsilon} dz$ to the Poisson equation (with $\epsilon \ll 1/k$). The left-hand side of the Poisson equation, after substituting the guessed solution, yields

$$\int_{-\epsilon}^{\epsilon} dz \nabla^2 \Phi = \partial_z \Phi|_{-\epsilon}^{\epsilon} = \Phi_a e^{ikx} (-2|k|).$$

The right-hand side gives

$$4\pi G\Sigma_a e^{ikx} \int_{-\epsilon}^{\epsilon} \delta_D(z) dz = 4\pi G\Sigma_a e^{ikx}.$$

Our guess is thus indeed a solution, and solving for Φ_a yields

$$\Phi = -\frac{2\pi G \Sigma_a}{|k|} e^{ikx - |kz|}. \quad (7.42)$$

Comparing this solution with Eq. (7.41), we can see that for a plane wave surface density Σ , the resulting Φ in the plane (i.e. at $z = 0$) equals Σ times $(-2\pi G/|k|)$. Since a radial wave looks locally (within a distance of a few wavelengths) like a Cartesian plane wave (i.e. we are again assuming the tight-winding approximation $kR \gg 1$), we can apply this to Eq. (7.37) to obtain

$$\Phi_1(R, \phi, t) \simeq -\frac{2\pi G}{|k|} H(R, t) e^{i[m\phi + f(R, t)]}. \quad (7.43)$$

7.3.7. Response of the disk to the potential

The final, and most elaborate, step of the derivation is to ensure that the perturbed potential affects the stellar orbits in a way that self-consistently corresponds to the spiral density wave. Here we will show this for the simpler case of a gas disk rather than a stellar disk.

7.3.7.1. Euler equation

We begin with the Euler equation as in Eq. (4.38), except that for a gas and with our present notation it is

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \vec{\nabla}) \vec{v} = -\frac{1}{\rho} \vec{\nabla} p - \vec{\nabla} \Phi. \quad (7.44)$$

In a disk, we set $z = 0$. Also, the pressure gradient term is

$$\frac{1}{\rho} \vec{\nabla} p = \frac{1}{\rho \Delta z} \vec{\nabla} (p \Delta z) \rightarrow \frac{1}{\Sigma} p,$$

where Δz is the thickness of the thin disk, the gradient is only applied inside the $z = 0$ plane, and we call $p \Delta z$ the two-dimensional pressure¹ and hereafter denote it simply p . Writing the Euler equation in cylindrical coordinates (see Eq. B.56 of [1]), the R and ϕ components are

$$\frac{\partial v_R}{\partial t} + v_R \frac{\partial v_R}{\partial R} + \frac{v_\phi}{R} \frac{\partial v_R}{\partial \phi} - \frac{v_\phi^2}{R} = -\frac{\partial \Phi}{\partial R} - \frac{1}{\Sigma} \frac{\partial p}{\partial R}, \quad (7.45)$$

$$\frac{\partial v_\phi}{\partial t} + v_R \frac{\partial v_\phi}{\partial R} + \frac{v_\phi}{R} \frac{\partial v_\phi}{\partial \phi} + \frac{v_\phi v_R}{R} = -\frac{1}{R} \frac{\partial \Phi}{\partial \phi} - \frac{1}{\Sigma R} \frac{\partial p}{\partial \phi}. \quad (7.46)$$

¹For a thin disk with a density that varies with z , the two-dimensional pressure is defined as $(\Sigma/\Delta z) \times \int (p/\rho) dz$.

We now assume the two-dimensional version of a simple (polytropic) equation of state (as for an adiabatic or isothermal gas),

$$p = K\Sigma^\gamma. \quad (7.47)$$

The speed of sound is then

$$c_s^2 = \frac{dp}{d\Sigma} = \gamma K\Sigma^{\gamma-1}. \quad (7.48)$$

Now we simplify the equations by using the (two-dimensional) specific enthalpy² h :

$$h \equiv \int \frac{dp}{\Sigma} = \int \frac{dp}{d\Sigma} \frac{d\Sigma}{\Sigma} = \int \gamma K\Sigma^{\gamma-2} d\Sigma = \frac{\gamma}{\gamma-1} K\Sigma^{\gamma-1} = \frac{c_s^2}{\gamma-1}. \quad (7.49)$$

We will need this result later, but for now, simply noting that $dh = dp/\Sigma$ simplifies the right-hand sides of Eq. (7.45) and Eq. (7.46), respectively, to:

$$-\frac{\partial}{\partial R}(\Phi + h) ; \quad -\frac{1}{R} \frac{\partial}{\partial \phi}(\Phi + h). \quad (7.50)$$

7.3.7.2. Unperturbed solution

Consider first the zeroth order, unperturbed solution. It is assumed to be axisymmetric and steady state, described by $\Sigma_0(R)$, $\Phi_0(R)$, and $h_0(R)$, corresponding to circular orbits so that $v_{R,0} = 0$ and [from Eq. (7.45) and Eq. (7.50)]

$$\frac{v_{\phi,0}^2}{R} = \frac{d}{dR}(\Phi_0 + h_0). \quad (7.51)$$

We now estimate the importance of the h_0 term. A circular orbit without pressure would be given by $V_c^2/R = d\Phi_0/dR$. Meanwhile, from Eq. (7.49), $dh_0/dR \sim c_s^2/R$. Thus, the relative contribution of the pressure term (in the Milky Way disk) is

$$\frac{c_s^2}{V_c^2} \sim \left(\frac{10 \text{ km/s}}{200 \text{ km/s}} \right)^2 \ll 1.$$

We conclude that we may approximately set $v_{\phi,0} \simeq V_c = R\Omega(R)$ and treat the correction to this as a first-order perturbation (which may be neglected when multiplying other first-order terms).

²We note that in three dimensions, the enthalpy is defined as $H = E + pV$, so $dH = (TdS - pdV) + d(pV) = TdS + Vdp$. If we assume $dS = 0$ and note that $V \propto 1/\rho$, then $H \propto \int dp/\rho$.

7.3.7.3. First-order Euler equation

We take Eq. (7.45) and Eq. (7.46), simplified with Eq. (7.50), and write them to first order about the just-noted unperturbed solution, after subtracting the zeroth order versions (which affects only the first equation). We obtain

$$\frac{\partial v_{R,1}}{\partial t} + \Omega \frac{\partial v_{R,1}}{\partial \phi} - 2\Omega v_{\phi,1} = -\frac{\partial}{\partial R}(\Phi_1 + h_1), \quad (7.52)$$

$$\frac{\partial v_{\phi,1}}{\partial t} + \left[\frac{d(\Omega R)}{dR} + \Omega \right] v_{R,1} + \Omega \frac{\partial v_{\phi,1}}{\partial \phi} = -\frac{1}{R} \frac{\partial}{\partial \phi}(\Phi_1 + h_1), \quad (7.53)$$

where in the first equation we used

$$v_\phi^2 = (v_{\phi,0} + v_{\phi,1})^2 \simeq v_{\phi,0}^2 + 2v_{\phi,0}v_{\phi,1}.$$

We want the solutions to correspond to spiral density waves, so we search for wave solutions of the form

$$v_{R,1} = v_{R,r}(R)e^{i(m\phi - \omega t)}, \quad (7.54)$$

where the physical solution is the real part. Here we have assumed the ϕ dependence needed for m spiral arms [compare Eq. (7.37)], assumed a wave in time, and left a general R -dependence for now (the R -dependent factor in the separation of variables is labeled with a subscript r , as opposed to subscript R which denotes a radial component of a vector). We assume the same wave form for the other relevant quantities: $v_{\phi,1}$, Φ_1 , h_1 , and Σ_1 . Note that the exponent of the wave is

$$i(m\phi - \omega t) \equiv im(\phi - \Omega_p t), \quad (7.55)$$

where Ω_p is the pattern speed, which describes the apparent angular speed of the spiral density pattern. As discussed in Sec. 7.3.1, this speed is in general different from that of stars within the spiral arm, since the arm does not correspond to fixed stars over time. Indeed, unlike Ω_p (which by definition does not depend on R), the stellar orbits generally display differential rotation (plus epicyclic motion, which corresponds to the velocity perturbation in the present case of a gas disk).

We substitute this wave solution into Eq. (7.52) and Eq. (7.53), and solve for the velocity components (a linear system of two equations in two unknowns). We obtain

$$v_{R,r} = \frac{-i}{\Delta} \left[(m\Omega - \omega) \frac{d}{dR}(\Phi_r + h_r) + \frac{2m\Omega}{R}(\Phi_r + h_r) \right], \quad (7.56)$$

$$v_{\phi,r} = \frac{1}{\Delta} \left[-2B \frac{d}{dR}(\Phi_r + h_r) + \frac{m(m\Omega - \omega)}{R}(\Phi_r + h_r) \right], \quad (7.57)$$

where

$$B(R) \equiv -\frac{1}{2} \left[\frac{d(\Omega R)}{dR} + \Omega \right] = -\Omega - \frac{1}{2} R \frac{d\Omega}{dR} \quad (7.58)$$

is the Oort B constant from Eq. (7.25), and the determinant is

$$\Delta = \kappa^2 - (m\Omega - \omega)^2, \quad (7.59)$$

where κ is given by Eq. (7.19) as before.

7.3.7.4. Other first-order equations

We have the **equation of state** in terms of the enthalpy in Eq. (7.49). To first order in the perturbation, this gives

$$h_1 = \gamma K \Sigma_0^{\gamma-2} \Sigma_1 = \frac{c_s^2(\Sigma_0)}{\Sigma_0} \Sigma_1. \quad (7.60)$$

Substituting the wave solution, we obtain

$$h_r = \frac{c_s^2(\Sigma_0)}{\Sigma_0} \Sigma_r. \quad (7.61)$$

Next is the **continuity equation** of Eq. (4.37), which in the present notation and in cylindrical coordinates (see Eq. B.47 of [1]) is

$$\frac{\partial \rho}{\partial t} + \frac{1}{R} \frac{\partial(R\rho v_R)}{\partial R} + \frac{1}{R} \frac{\partial(\rho v_\phi)}{\partial \phi} + \frac{\partial(\rho v_z)}{\partial z} = 0. \quad (7.62)$$

For a thin disk, we multiply by the thickness Δz , assume v_z is negligible, and note that to first order:

$$\rho v_R \Delta z = \Sigma v_R \simeq \Sigma_0 v_{R,1}; \quad \partial_\phi(\Sigma v_\phi) \simeq (\partial_\phi \Sigma_1) R \Omega + \Sigma_0 \partial_\phi v_{\phi,1}.$$

The continuity equation to first order (note that it is trivial to zeroth order) is then

$$\frac{\partial \Sigma_1}{\partial t} + \frac{1}{R} \frac{\partial}{\partial R} (R \Sigma_0 v_{R,1}) + \Omega \frac{\partial \Sigma_1}{\partial \phi} + \frac{\Sigma_0}{R} \frac{\partial v_{\phi,1}}{\partial \phi} = 0. \quad (7.63)$$

Substituting the wave solution yields:

$$i(m\Omega - \omega)\Sigma_r + \frac{1}{R} \frac{d}{dR} (R \Sigma_0 v_{R,r}) + \frac{im\Sigma_0}{R} v_{\phi,r} = 0. \quad (7.64)$$

At this point it is useful to sum up where we are. We have four equations (two Euler components, the equation of state, and continuity), but five unknowns ($v_{R,r}$, $v_{\phi,r}$, Φ_r , h_r , and Σ_r). It remains to include the **Poisson** equation. This is given by Eq. (7.43) along with Eq. (7.35), except that in the wave solution we have separated out the time-dependence. Thus, the radial dependence in Eq. (7.37) is

$$\Sigma_r(R) = H(R) e^{if(R)}, \quad (7.65)$$

where H is smooth while f varies rapidly, and the solution to the Poisson equation is

$$\Phi_r = -\frac{2\pi G}{|k|}\Sigma_r, \quad (7.66)$$

where $k \equiv df/dR$.

7.3.7.5. Final equations

We now use the tight-winding approximation ($kR \gg 1$) for one final round of simplification. With Σ_r as in Eq. (7.65), we note that since only f varies rapidly, a radial derivative simply multiplies by the factor ik . The same is also true for Φ_r [using Eq. (7.66)] and for h_r [using Eq. (7.61)]. In the components of the Euler equation [Eq. (7.56) and Eq. (7.57)], the terms on the right-hand side with a radial derivatives are larger than the terms that have a $1/R$ factor, by $\sim kR$; thus, the latter can be neglected, giving

$$v_{R,r} = \frac{k}{\Delta}(m\Omega - \omega)(\Phi_r + h_r), \quad (7.67)$$

$$v_{\phi,r} = -\frac{2i}{\Delta}Bk(\Phi_r + h_r). \quad (7.68)$$

Similarly, in the continuity equation of Eq. (7.64), the last term is smaller than the middle term by $\sim 1/(kR)$ (since, from the just-written Euler equation, $v_{R,r}$ and $v_{\phi,r}$ are of similar amplitude), so we obtain

$$(m\Omega - \omega)\Sigma_r + k\Sigma_0 v_{R,r} = 0. \quad (7.69)$$

The final linear system of five equations in five unknowns consists of the Euler [Eq. (7.68) and Eq. (7.67)], continuity [Eq. (7.69)], and Poisson [Eq. (7.66)] equations, plus the equation of state [Eq. (7.61)].

7.4. Spiral structure: result

7.4.1. Basic solution

Solving the equations in Sec. 7.3.7.5 leads to

$$v_{R,r} = \frac{1}{\Delta}(m\Omega - \omega)k\Sigma_r \left(\frac{c_s^2}{\Sigma_0} - \frac{2\pi G}{|k|} \right). \quad (7.70)$$

Thus, the continuity equation [Eq. (7.69)] yields

$$(m\Omega - \omega)\Sigma_r \left(1 + \frac{k^2 c_s^2}{\Delta} - \frac{2\pi G \Sigma_0 |k|}{\Delta} \right) = 0. \quad (7.71)$$

This solution breaks down (or becomes degenerate) at special points (i.e. radii). First, as noted in Sec. 7.3.7.3, $\Omega_p \equiv \omega/m$ is the angular speed of the spiral arm

pattern, while Ω is the speed of the stellar guiding center (or the zeroth order velocity, in the present case of a gas disk). One of the special points is where

$$\Omega = \Omega_p. \quad (7.72)$$

This is called the *corotation resonance*. Its physical meaning is that at this radius, stars rotate along with the spiral pattern, so each star feels a constant (rotating) gravitational force from the spiral perturbation. Over time, this resonant force can produce large displacements. However, this resonance is expected to be somewhat smoothed out and tempered by the epicycles (i.e. the velocity perturbation with respect to constant circular motion).

More serious is the singularity at $\Delta = 0$. Remembering Eq. (7.59), the singularity occurs at

$$\pm \kappa = m\Omega - \omega = m(\Omega - \Omega_p), \quad (7.73)$$

or equivalently, $\Omega_p = \Omega \mp (\kappa/m)$. Recall that κ is the epicyclic angular speed, and note that $\Omega - \Omega_p$ is the speed of the guiding center relative to the spiral arm pattern. The two solutions are called the *Lindblad resonances*, specifically the inner (corresponding to the minus sign) and outer (corresponding to the plus sign) Lindblad resonances. To see the physical meaning, note that the singularity condition is equivalent to

$$\frac{2\pi}{\kappa} = \frac{1}{m} \frac{2\pi}{|\Omega - \Omega_p|},$$

which means that the epicyclic period is equal to the period when the guiding center crosses a spiral arm, and gets a gravitational impulse from the increased density of the arm. The resonance occurs when impulses repeat at the same point in the epicyclic motion, and thus add constructively over time.

Due to this singularity, spiral arms are expected only between the Lindblad resonances. In this range of radii, the epicyclic period is shorter than the period for crossing a spiral arm, so intuitively, there is enough time for the stellar orbits to react to the spiral arms in a way that maintains the spiral density wave. We also note that the corotation resonance occurs somewhere within the range of the spiral structure, between the two Lindblad resonances.

Real spiral structure as observed in galaxies varies in terms of the number of arms, the angular extent of each arm, and the degree to which the arms are clearly delineated and well formed. A spectacular example is shown in Fig. 7.3.

7.4.2. Dispersion relation

Away from the problematic points, Eq. (7.71) gives the following dispersion relation:

$$(m\Omega - \omega)^2 = \kappa^2 - 2\pi G\Sigma|k| + k^2 c_s^2, \quad (7.74)$$



Fig. 7.3. A Hubble space telescope image of the spiral galaxy M51. A prominent $m = 2$ spiral-arm pattern is apparent, with relatively tightly wound arms that extend over at least 450° . The gravitational perturbation from the companion (NGC 5195) may have helped trigger this spectacular spiral pattern. Credit: NASA, ESA, STScI, AURA, S. Beckwith, Hubble Heritage Team.

where we have suppressed the subscript on Σ_0 . The result for a stellar disk has a similar form, but is mathematically more involved (Eq. 6.61 of [1]):

$$(m\Omega - \omega)^2 = \kappa^2 - 2\pi G\Sigma|k| + \mathcal{F}\left(\frac{\omega - m\Omega}{\kappa}, \frac{k^2\sigma_R^2}{\kappa^2}\right), \quad (7.75)$$

where $\mathcal{F}$ is a complicated integral, and the stellar radial velocity dispersion σ_R essentially plays the same role as the speed of sound in the case of a gas disk.

Before discussing the consequences of this result, we again note that it has a number of important limitations. It is only a local (and linear) solution, while an accurate global solution would require detailed consideration of the effect of the singularities/resonances discussed in the previous subsection; adding the disk boundary conditions (at the center and at the edge of the disk); and relaxing some of the approximations that we made, in particular the tight-winding approximation. Further derivations and extended discussion can be found in Chap. 6 of [1].

7.4.3. Stability

The key result of the derivation in this section is that a spiral density wave solution indeed exists. However, there is another central consequence of the dispersion relation presented in the previous subsection: gravitational instability in disks.

We consider the simple case of axisymmetric disturbances ($m = 0$), for which the above derivation remains valid as long as $|kR| \gg 1$. Equation 7.74 then gives ω^2 as a parabolic function of $|k|$, where the time dependence of the solution is $\Sigma_1 \propto \exp(-i\omega t)$. Stability is ensured if the time evolution is oscillatory (and not exponentially growing), i.e. if $\omega^2 > 0$ for *all* values of $|k|$; a random perturbation will typically consist of contributions from many different k values, and if even one of them were to grow exponentially, it would make the perturbation unstable. The parabola (which is concave up) is always positive if the discriminant is negative³:

$$(2\pi G\Sigma)^2 - 4\kappa^2 c_s^2 < 0, \quad (7.76)$$

which is equivalent to the stability condition

$$Q_{\text{gas}} \equiv \frac{c_s \kappa}{\pi G \Sigma} > 1. \quad (7.77)$$

This is known as the *Toomre stability criterion* [4, 5]. The result for a stellar disk is similar [5]:

$$Q_{\text{stars}} \equiv \frac{\sigma_R \kappa}{3.36 G \Sigma} > 1. \quad (7.78)$$

This stability analysis provides a key insight into the gravitational instability that leads to star formation in disks (although that process is very complex and also involves other types of physics such as magnetic fields). From this criterion, it can be seen that gravity (as in high Σ) promotes instability (which leads to high density and facilitates star formation), while a large internal velocity (as measured by c_s or σ_R , as appropriate) tends to spread out density structures and prevent gravitational collapse. Indeed, this is reminiscent of the Jeans instability analysis of Sec. 4.5.5. In the Jeans case, for a gas we had stability if the velocity induced by gravity was smaller than the speed of sound, in which case pressure can act quickly enough to counteract gravity. In the disk case, the typical velocity induced by gravity is the

³Letting $x = |k|$, the minimum of the parabola versus x is always at positive x , so the absolute value does not change the result.

circular velocity

$$V_c \sim \sqrt{\frac{GM}{R}} \sim \sqrt{\frac{G\Sigma R^2}{R}} \sim \sqrt{G\Sigma R},$$

and since $\kappa \sim \Omega \sim V_c/R$, the Q parameter is

$$Q \sim \frac{c_s \kappa}{G\Sigma} \sim \frac{c_s V_c}{G\Sigma R} \sim \frac{c_s V_c}{V_c^2} \sim \frac{c_s}{V_c}.$$

Thus, $Q > 1$ gives stability, as it corresponds to pressure winning in its contest with gravity.

Finally, we note that spiral arms are often so visually prominent because the associated small density enhancement can strongly enhance star formation. The fact that stability is characterized by a *threshold* means that star formation can be very sensitive to small changes (in density or velocity dispersion) that push a region beyond the threshold into instability (This idea is similar in spirit to biased galaxy formation, whereby regions with a small overdensity of matter can have a large overdensity in the number of galaxies; see Sec. 3.4.3 and Sec. 11.2). More generally, the response of various populations to the spiral density wave depends on the ratio of the velocity dispersion of the population to the typical gravitational velocity induced by the density perturbation. In a galaxy such as the Milky Way, halo stars have a velocity dispersion above 100 km/s, disk stars are around 30 km/s, and the gas clouds in the disk (where stars form) are much “colder”, in the sense that their velocity dispersion is ~ 10 km/s. Thus, the small density perturbation associated with a spiral arm can have no effect on the distribution of halo stars, a mild effect on disk stars, and a large effect on gas clouds, with the latter inducing the formation of bright young stars that light up the spiral arms for astronomers to see and enjoy.

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Chapter 8

Gravitational Lensing

Gravitational lensing is a subject that has a wide range of applications in cosmology and astrophysics. Strong lensing (in which there are large lensing distortions and multiply-imaged sources) is used to measure the masses of galactic halos (and cluster cores) and probe their substructure. Weak lensing is used to determine the mass distribution of galaxy clusters and of large-scale structure on cosmological scales. Microlensing is used to find otherwise undetectable stars and planets. There is a book on lensing [1] and many reviews. In this chapter we give a brief introduction to the subject.

8.1. The lens equation

We begin with a point-mass as the lens. We utilize from general relativity Einstein's famous result for the light bending (or deflection) angle γ due to a mass M , for light passing at a closest distance r from the deflecting mass:

$$\gamma = \frac{4GM}{c^2 r}. \quad (8.1)$$

In particular, for light passing near the sun (as in Eddington's historic test of general relativity in 1919),

$$\frac{4GM_{\odot}}{c^2 R_{\odot}} = 1''.74.$$

We assume the *thin lens approximation*, whereby the deflection mostly occurs near the lens, at distances from the lens that are much smaller than the distance of the lens to the observer or to the source. In this case, the deflection can be approximated as occurring at a point, giving a simple basic geometry for lensing as shown in Fig. 8.1. In the cosmological context (assuming a flat universe), this diagram is valid in comoving coordinates. Note that the observer, lens, and source

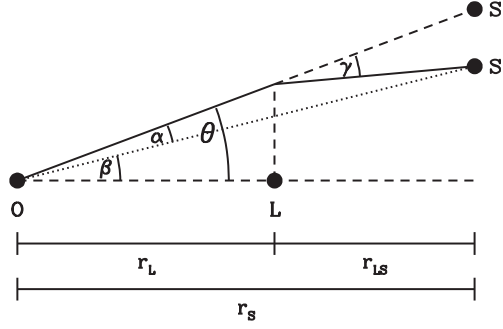


Fig. 8.1. Schematic drawing showing the basic geometry of the lens equation, in the thin lens approximation. We show the observer O , lens L , and source S . In the absence of lensing, the observer would be seen at an angular position β with respect to the lens. However, the deflection angle γ causes the source to appear at the apparent image angle θ . It is useful to also define the scaled deflection angle α . The relevant distances are r_L (observer-lens, also commonly denoted r_{OL}), r_{LS} (lens-source), and r_S (observer-source, also commonly denoted r_{OS}). In cosmology these are comoving distances to a lens at redshift z_L and a source at redshift z_S , and we assume a flat spatial geometry.

(O-L-S) positions together determine a plane, and the deflection occurs in that plane (so that the entire diagram is drawn in that plane).

The lens equation is simply $\alpha + \beta = \theta$, but it is usually written as

$$\beta = \theta - \alpha(\theta), \quad (8.2)$$

so that for a given lensing mass [giving the function $\alpha(\theta)$] and source position β , this equation is to be solved to give the image position(s) θ . In astrophysical cases of gravitational lensing, the deflection angles are usually very small (arcseconds or at most a few arcminutes), so that we can make small-angle approximations such as $\sin \alpha \simeq \tan \alpha \simeq \alpha$. Thus, $\alpha r_S = \gamma r_{LS}$, in terms of the comoving observer-source and lens-source distances. It is more common to use angular diameter distances, which relate observed angles to proper (physical) distances; then we have the observer-source [$D_S = r_S/(1+z_S)$], observer-lens [$D_L = r_L/(1+z_L)$], and lens-source [$D_{LS} = r_{LS}/(1+z_S)$] distances. Therefore, the lens equation can be written as

$$\beta = \theta - \frac{D_{LS}}{D_S} \gamma. \quad (8.3)$$

For a point mass, γ is given by Eq. (8.1), where r is the proper distance in the lens plane (i.e. the impact parameter of the light ray with respect to the lens), written as ξ and given by

$$\xi = D_L \theta. \quad (8.4)$$

Thus, in this case

$$\alpha(\theta) = \frac{D_{LS}}{D_S} \frac{4GM}{c^2 D_L \theta} = \frac{4GM}{c^2} \frac{D_{LS}}{D_S D_L} \frac{1}{\theta} \equiv \frac{\theta_E^2}{\theta}, \quad (8.5)$$

where we have defined the *Einstein radius*

$$\theta_E = \sqrt{\frac{4GM}{c^2} \frac{D_{LS}}{D_S D_L}} \sim 3'' \left(\frac{M}{10^{12} M_\odot} \right)^{1/2} \left[\frac{D_{LS}/(D_S D_L)}{1/\text{Gpc}} \right]^{1/2}. \quad (8.6)$$

This angle gives the characteristic scale for the angular separation of lensed images of a source. For a lens galaxy of mass $M \sim 10^{12} M_\odot$, and cosmological distances (of order a Gpc), θ_E is several arcseconds. If the lensing mass is a galaxy cluster with $M \sim 10^{15} M_\odot$, the scale becomes a few arcminutes.

8.2. Point-mass lens

From the previous section, the lens equation for a point-mass lens is

$$\beta = \theta - \frac{\theta_E^2}{\theta}. \quad (8.7)$$

This is a quadratic equation for θ , with solutions

$$\theta_{\pm} = \frac{1}{2} \left(\beta \pm \sqrt{\beta^2 + 4\theta_E^2} \right) = \frac{\theta_E}{2} \left(u \pm \sqrt{u^2 + 4} \right), \quad (8.8)$$

where $u = \beta/\theta_E$ is the (actual) source position in units of θ_E . A special case is $u = 0$, for which Eq. (8.8) gives $\theta = \pm\theta_E$; however, in that case (where the source lies directly behind the lens) there is azimuthal symmetry with respect to the observer-lens-source axis, and the image is a full ring of radius θ_E (an *Einstein ring*). In the limit of $u \rightarrow \infty$ (a source that is far off-axis), the two solutions are $u = \beta$ (the original source) and $u = 0$. There is always a second image in this case, because the deflection angle diverges as $\theta \rightarrow 0$.

A basic result in general relativity is that surface brightness is conserved under gravitational lensing (e.g. [1]). Thus, the magnification μ is equal to the ratio of angular areas:

$$\mu = \left| \frac{\theta d\theta}{\beta d\beta} \right|, \quad (8.9)$$

where θ/β is the tangential magnification (perpendicular to the O-L-S plane) and $d\theta/d\beta$ is the radial magnification (in the O-L-S plane, perpendicular to the line of sight). For the point-mass lens, this comes out as

$$\mu_{\pm} = \frac{u^2 + 2}{2u\sqrt{u^2 + 4}} \pm \frac{1}{2}. \quad (8.10)$$

The total magnification is

$$\mu_{\text{tot}} = \mu_+ + \mu_- = \frac{u^2 + 2}{u\sqrt{u^2 + 4}} > 1, \quad (8.11)$$

where the last inequality can easily be seen by squaring the numerator and the denominator. At $u \rightarrow 0$, $\mu_{\text{tot}} \rightarrow \infty$, as the point source is stretched into a ring

(which corresponds to infinite tangential magnification). At $u \rightarrow \infty$, $\mu_+ = 1$ (the original source appears essentially unchanged) while $\mu_- = 0$ (the counter-image is strongly demagnified). We note that the always-positive magnification ($\mu_{\text{tot}} > 1$) is true only in the small-angle approximation.

8.3. General lens

More generally, if the lensing is due to a distribution of mass, all located in the same vicinity (to within a distance that is much smaller than D_L or D_{LS}), then the entire lensing mass distribution can be projected onto a single lens plane (perpendicular to the observer-lens line of sight), and the total deflection angle is the sum of the deflection angles of the individual masses in the lens, each determined by its mass and its impact parameter (i.e. the distance in the lens plane between the light ray position $\vec{\xi}$ and the position $\vec{\xi}'$ of the mass). In this case, the lens equation is a vector equation, with vector angles (two-dimensional vectors) that measure the angular position in a plane perpendicular to the observer-lens line of sight (where the “lens” is simply a fiducial position in the lens plane, fixed as the origin of the angular coordinates):

$$\vec{\beta} = \vec{\theta} - \vec{\alpha}(\vec{\theta}), \quad (8.12)$$

where

$$\vec{\alpha} = \frac{D_{LS}}{D_S} \vec{\gamma}, \quad (8.13)$$

and

$$\vec{\gamma} = \sum \frac{4GM(\vec{\xi}')}{c^2} \frac{\vec{\xi} - \vec{\xi}'}{|\vec{\xi} - \vec{\xi}'|^2} = \frac{4G}{c^2} \int \frac{\vec{\xi} - \vec{\xi}'}{|\vec{\xi} - \vec{\xi}'|^2} \Sigma(\vec{\xi}') d^2\xi'. \quad (8.14)$$

Here, in the first step we wrote a discrete sum over point masses, and in the second step we transitioned to the continuous limit of a surface mass density Σ projected onto the lens plane. Using $\vec{\xi} = D_L \vec{\theta}$, we obtain

$$\vec{\alpha} = \frac{D_{LS} D_L}{D_S} \frac{4G}{c^2} \int \frac{\vec{\theta} - \vec{\theta}'}{|\vec{\theta} - \vec{\theta}'|^2} \Sigma(\vec{\theta}') d^2\theta' = \frac{1}{\pi} \int \frac{\vec{\theta} - \vec{\theta}'}{|\vec{\theta} - \vec{\theta}'|^2} \kappa(\vec{\theta}') d^2\theta', \quad (8.15)$$

where

$$\kappa \equiv \Sigma / \Sigma_{\text{cr}}, \quad (8.16)$$

in terms of the characteristic *critical surface density*

$$\Sigma_{\text{cr}} = \frac{D_S}{D_L D_{LS}} \frac{c^2}{4\pi G} \sim 0.4 \left[\frac{D_S / (D_L D_{LS})}{1/\text{Gpc}} \right] \text{g/cm}^2. \quad (8.17)$$

It happens that the characteristic surface density for cosmological lensing is of order a gram per square cm. Now, noting that in two dimensions

$$\vec{\nabla}_\theta \ln \theta = \frac{1}{\theta^2} \vec{\theta}, \quad (8.18)$$

the (scaled) deflection angle can be written as the (two-dimensional angular) gradient of a two-dimensional potential:

$$\vec{\alpha} = \vec{\nabla} \psi, \quad (8.19)$$

where

$$\psi = \frac{1}{\pi} \int \kappa(\vec{\theta}') \ln |\vec{\theta} - \vec{\theta}'| d^2 \theta'. \quad (8.20)$$

Consider now the (two-dimensional angular) Laplacian of $\ln \theta$. Using polar coordinates (θ, ϕ) for $\vec{\theta}$ (where the radial coordinate normally denoted R is here the magnitude θ),

$$\nabla_\theta^2 \ln \theta = \frac{1}{\theta} \frac{\partial}{\partial \theta} \left(\theta \frac{\partial}{\partial \theta} \ln \theta \right) = 0, \quad (8.21)$$

if $\theta \neq 0$. On the other hand, if we integrate this quantity over a circular area A centered at the origin, we obtain

$$\int_A \nabla_\theta^2 (\ln \theta) d^2 \theta = \int_A \vec{\nabla} \cdot \vec{\nabla} (\ln \theta) d^2 \theta = \int_A \vec{\nabla} \cdot \left(\frac{1}{\theta^2} \vec{\theta} \right) d^2 \theta,$$

where we used Eq. (8.18). We now use the two-dimensional version of the divergence theorem to equate this to a line integral over the boundary of the area (i.e. a circle C whose center is at the origin):

$$\int_A \nabla_\theta^2 (\ln \theta) d^2 \theta = \oint_C \left(\frac{1}{\theta^2} \vec{\theta} \right) \cdot \hat{\theta} \theta d\phi = \frac{1}{\theta} (2\pi\theta) = 2\pi. \quad (8.22)$$

The combination of Eq. (8.21) and Eq. (8.22) implies that

$$\nabla_\theta^2 (\ln \theta) = 2\pi \delta_D \left(\vec{\theta} \right). \quad (8.23)$$

Then together with Eq. (8.20) we obtain

$$\nabla^2 \psi = \frac{1}{\pi} \int \kappa(\vec{\theta}') \delta_D \left(\vec{\theta} - \vec{\theta}' \right) d^2 \theta' = 2\kappa(\vec{\theta}). \quad (8.24)$$

We note from Eq. (8.19) that this also equals the divergence of $\vec{\alpha}$, whereas its curl is zero. We see that the lensing potential ψ is determined by a two-dimensional Poisson equation, and $\vec{\alpha}$ is determined by κ in a mathematically similar way (except in two dimensions rather than three) as the Newtonian gravitational force is determined by the mass distribution.

8.4. Magnification and shear

In the general lensing case of the previous section, the magnification is determined by the Jacobian matrix of the $\vec{\beta} \rightarrow \vec{\theta}$ mapping, which gives the mapping of areas from the source plane to the image plane. The Jacobian matrix is

$$A = \frac{\partial \beta_i}{\partial \theta_j} = \delta_{ij} - \frac{\partial \alpha_i}{\partial \theta_j} = \delta_{ij} - \frac{\partial^2 \psi}{\partial \theta_i \partial \theta_j} = \delta_{ij} - \psi_{ij} = \begin{pmatrix} 1 - \psi_{11} & -\psi_{12} \\ -\psi_{21} & 1 - \psi_{22} \end{pmatrix}, \quad (8.25)$$

where i, j are indices that run over the two dimensions 1 and 2, ψ_{ij} is short-hand for the second-order partial derivatives of ψ , and in the final step we wrote out the 2×2 matrix. The magnification matrix is then

$$M = A^{-1}, \quad (8.26)$$

and the magnification equals

$$\mu = \det M = \frac{1}{\det A}. \quad (8.27)$$

The Jacobian matrix can also be expressed in an alternative way, by first noticing from Eq. (8.24) that

$$\kappa = \frac{1}{2} (\psi_{11} + \psi_{22}) = \frac{1}{2} \text{tr } \psi_{ij}. \quad (8.28)$$

The other components (in addition to the trace) can be described with the two parameters

$$\gamma_1 \equiv \frac{1}{2} (\psi_{11} - \psi_{22}) \equiv \gamma \cos(2\phi), \quad (8.29)$$

and

$$\gamma_2 \equiv \psi_{12} = \psi_{21} \equiv \gamma \sin(2\phi). \quad (8.30)$$

Here we first defined (γ_1, γ_2) and then transformed to (γ, ϕ) just like polar coordinates (except using 2ϕ instead of ϕ). Then we can write

$$A = \begin{pmatrix} 1 - \kappa - \gamma_1 & -\gamma_2 \\ -\gamma_2 & 1 - \kappa + \gamma_1 \end{pmatrix} = (1 - \kappa) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \gamma \begin{pmatrix} \cos 2\phi & \sin 2\phi \\ \sin 2\phi & -\cos 2\phi \end{pmatrix}, \quad (8.31)$$

and

$$\mu = \frac{1}{(1 - \kappa)^2 - \gamma^2}. \quad (8.32)$$

The *convergence* κ on its own corresponds to a straight magnification of a source without a change of shape, while the *shear* on its own corresponds to a distortion

that stretches a circular source into an elliptical image with a major axis at an angle ϕ .

8.5. Axisymmetric lens

When the mass distribution, projected onto the lens plane, is axisymmetric (about a point where we set the origin), the lens geometry simplifies. By symmetry, the deflection angle in this case is in the plane containing the observer, lens center, and source, so the lens equation is one-dimensional as in the point-mass lens of Sec. 8.2. Moreover, similarly to the three-dimensional case, the two-dimensional version of Gauss's Law (or divergence theorem) applied to $\vec{\alpha}$ [based on Eq. (8.24)] implies that the deflection angle is like that of a point-mass lens (Sec. 8.2) but depends on the enclosed projected mass $M(\xi)$ out to projected radius ξ , i.e.

$$\gamma = \frac{4GM(\xi)}{c^2\xi}, \quad (8.33)$$

where

$$M(\xi) = \int_0^\xi \Sigma(\xi') 2\pi\xi' d\xi'. \quad (8.34)$$

The lens equation in this case is

$$\beta = \theta - \frac{4G}{c^2} \frac{D_{LS}}{D_S D_L} \frac{M(\theta)}{\theta}. \quad (8.35)$$

Just as for the point-mass lens, in the more general axisymmetric case a source at $\beta = 0$ produces an Einstein ring of radius defined to be the Einstein radius θ_E . The mean projected surface density within the Einstein radius is seen to equal

$$\bar{\Sigma} = \frac{M(\theta_E)}{\pi(D_L\theta_E)^2} = \frac{c^2 D_S D_L / (4G D_{LS})}{\pi D_L^2} = \frac{c^2 D_S}{4\pi G D_L D_{LS}} = \Sigma_{\text{cr}}. \quad (8.36)$$

This is an important property of the critical surface density.

8.6. The singular isothermal sphere lens

As a specific example of the axisymmetric lens discussed in the previous section, we consider the SIS of Sec. 6.6.2. The SIS mass distribution is the simplest reasonable approximation for a dark matter halo, so the SIS is often the starting point for modeling the lensing mass distribution of a galaxy or a cluster. The projected mass [Eq. (6.51)] is

$$\Sigma(\xi) = \frac{\sigma^2}{2G\xi},$$

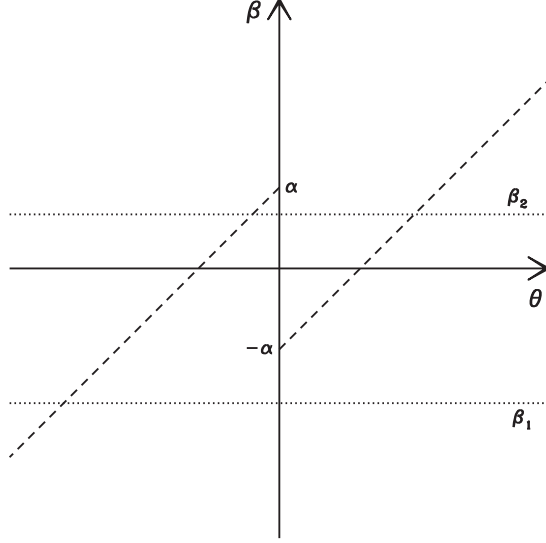


Fig. 8.2. Plot of the lens equation for an SIS lens. For a given source position β , the intersection of a horizontal line at β (dotted curves) with the lens-equation curve $\beta(\theta)$ (dashed curve) yields the image positions. We illustrate this with two example source positions: β_1 (for which there is a single image) and β_2 (for which there are two images of the source).

so the projected mass enclosed within radius ξ is

$$M(\xi) = \int_0^\xi \frac{\sigma^2}{2G\xi'} 2\pi\xi' d\xi' = \frac{\pi\sigma^2}{G}\xi. \quad (8.37)$$

The deflection angle is constant with radius:

$$\gamma = 4\pi \frac{\sigma^2}{c^2}; \quad \alpha = \frac{D_{LS}}{D_S} \gamma = \frac{1}{\Sigma_{\text{cr}}} \frac{\sigma^2}{GD_L}. \quad (8.38)$$

Since the deflection is always towards the lens center, the lens equation in this case is

$$\beta = \theta - \alpha \text{sign}(\theta). \quad (8.39)$$

As is easily seen from a $\beta(\theta)$ plot [see Fig. 8.2], there are two images when $|\beta| < \alpha$, at $\theta_\pm = \beta \pm \alpha$. When $|\beta| > \alpha$ there is a single image (at $\theta = \beta + \alpha \text{sign}(\beta)$). The Einstein radius of this lens is $\theta_E = \alpha$.

The magnification of an image of the SIS lens is [using Eq. (8.9), which is valid for any axisymmetric lens]

$$\mu = \left| \frac{\theta d\theta}{\beta d\beta} \right| = \left| \frac{\beta \pm \theta_E}{\beta} \right| = \left| 1 \pm \frac{1}{u} \right|, \quad (8.40)$$

where $u = \beta/\theta_E$. In particular, when $u \rightarrow 0$ (the Einstein ring limit), μ diverges as $1/u$, while when $u \rightarrow \infty$ (which corresponds to a distant source with a single image), $\mu \rightarrow 1$. We note that while the example mass distributions that we have



Fig. 8.3. Hubble telescope image of the galaxy cluster Abell 2218. This rich galaxy cluster contains thousands of galaxies (of which the largest ones are seen in yellow). The cluster halo gravitationally lenses many background galaxies, magnifying and distorting some of them into prominent arcs. The arcs trace out partial Einstein rings, whose sizes can be used to estimate the enclosed projected mass within the cluster. The detailed arc pattern is complex, as the individual galaxies contribute to the lensing potential on top of the overall, relatively smooth, cluster halo. Credit: NASA, ESA, and Johan Richard (Caltech, USA).

considered in this chapter (a point mass and an SIS) are both singular (i.e. $\Sigma(\xi)$ diverges at their center), in general, any non-singular lens has an odd number of images (e.g. [1]). A famous example of gravitational lensing is shown in Fig. 8.3.

8.7. The time delay and Fermat's principle

The general lens equation [Eq. (8.12)], with the help of Eq. (8.19), is

$$\vec{\beta} = \vec{\theta} - \vec{\nabla}\psi. \quad (8.41)$$

This is equivalent to

$$0 = \vec{\theta} - \vec{\beta} - \vec{\nabla}\psi = \vec{\nabla}_{\theta} \left[\frac{1}{2} |\vec{\theta} - \vec{\beta}|^2 - \psi \right]. \quad (8.42)$$

Thus, solving the lens equation can also be seen as finding the light path to the source (through the lens plane at a position given by $\vec{\theta}$) that minimizes the quantity

in square brackets; more precisely, the solution is an extremum of this quantity with respect to changing the path (by changing $\vec{\theta}$). This quantity turns out to be (proportional to) the time delay. Here we derive the geometrical time delay due to the increased path length of the actual light path (including lensing) compared to a straight line to the source (which would be the path in the absence of lensing).

We refer to the lensing diagram of Fig. 8.1, but generalize the expressions to a lens that might not be axisymmetric. We assume the FRW metric of Sec. 2.1.1 in a flat ($k = 0$) universe, and use comoving coordinates (with r for radial distance) and comoving time τ . For a light ray, $ds = 0$ so that $\Delta\tau$ equals the comoving distance. In a flat universe, the calculation of comoving distances from radial and angular components is Euclidean. Using the small-angle approximation, in the unlensed case

$$\Delta\tau(\text{unlensed}) = r_S \sqrt{1 + \beta^2} \simeq r_S \left(1 + \frac{1}{2}\beta^2\right),$$

while the lensed case consists of two segments:

$$\Delta\tau(\text{lensed}) \simeq r_L \left(1 + \frac{1}{2}\theta^2\right) + r_{LS} \left(1 + \frac{1}{2}|\vec{\theta} - \vec{\gamma}|^2\right).$$

Here $\vec{\theta}$ is the direction to the image with respect to the observer-lens direction, and $\vec{\gamma}$ is the difference between this direction and the actual direction of the light ray in the second segment, so that their difference is the direction of the second segment with respect to the observer-lens direction. Thus, the time difference measured at present (which is equal to the comoving time difference) is

$$\Delta t = \frac{1}{2}r_{LS} |\vec{\theta} - \vec{\gamma}|^2 + \frac{1}{2}r_L\theta^2 - \frac{1}{2}r_S\beta^2. \quad (8.43)$$

We now use the lens equation [Eq. (8.12)] to see that

$$\vec{\theta} - \vec{\gamma} = \vec{\theta} - \frac{r_S}{r_{LS}}\vec{\alpha} = \vec{\theta} - \frac{r_S}{r_{LS}}(\vec{\theta} - \vec{\beta}) = \frac{r_S\vec{\beta} - r_L\vec{\theta}}{r_{LS}}.$$

Thus,

$$\Delta t = \frac{1}{2} \left[\theta^2 \left(\frac{r_L^2}{r_{LS}} + r_L \right) + \beta^2 \left(\frac{r_S^2}{r_{LS}} - r_S \right) - 2\vec{\theta} \cdot \vec{\beta} \frac{r_L r_S}{r_{LS}} \right] = \frac{1}{2} \frac{r_L r_S}{r_{LS}} |\vec{\theta} - \vec{\beta}|^2.$$

Now we use $D_L = a_L r_L$, $D_{LS} = a_S r_{LS}$, and $D_S = a_S r_S$ (where a is the scale factor) to find the final expression for the geometric time delay:

$$\Delta t = \frac{1}{2} \frac{D_L D_S}{a_L D_{LS}} |\vec{\theta} - \vec{\beta}|^2. \quad (8.44)$$

To this must be added the gravitational time delay, the effect in general relativity of the slowing down of time in a gravitational potential compared to a distant observer. Also called the Shapiro time delay [2], in the thin-lens approximation it is proportional to the two-dimensional potential ψ (e.g. [1]). Inserting the speed of

light (which we have previously set to unity) and using the lens redshift z_L , the total lensing time delay is

$$\Delta t = \frac{1+z_L}{c} \frac{D_L D_S}{D_{LS}} \left[\frac{1}{2} \left| \vec{\theta} - \vec{\beta} \right|^2 - \psi(\vec{\theta}) \right]. \quad (8.45)$$

Thus, as shown at the beginning of this section, the lens equation is equivalent to finding the light path from the observer to the source that passes, at the lens plane, at the position that minimizes the arrival time. This is an example of Fermat's principle, or *the principle of least time*, which is used in classical optics and in quantum electrodynamics, and is also valid in general relativity.

When the emitted intensity of a multiply-imaged source varies with time, the same variation can be seen at different times in the different images, according to the relative time delays of the different paths taken by the light to come to us from the same source. Such a time measurement gives an absolute scale, and can thus be used to directly infer cosmological distances and thus constrain cosmological parameters such as the Hubble constant [3]. The first gravitational lens (the doubly-imaged quasar Q0957+561) was discovered in 1979 [4] and a few years later became the first lensing system with a measured time delay [5]. Since then, time delays have been measured in many more systems, but their use for cosmology is complicated by the need to reconstruct the lensing mass distribution accurately.

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Chapter 9

Summary and Conclusions

In part I we have laid out the basic understanding of galaxies in modern cosmology. We focused on several main topics. One of them is the power spectrum of density fluctuations, which is the key statistical quantity in cosmology, which in particular determines the distribution of galactic halos. Since the early Universe was highly uniform, linear perturbation theory is a natural framework for understanding the evolution of the power spectrum from the initial density fluctuations, perhaps produced during an early period of cosmic inflation, to its present form roughly in the shape of a broken power law. In the late, non-linear regime, collapse and virialization are the principal concepts in the formation of halos. The former is illustrated by the detailed, analytically tractable example of spherical collapse, while the latter can be analyzed using the virial theorem. These various concepts come together in the Press–Schechter model which yields a quantitative understanding of the connection between the initial fluctuations and the final distribution of massive virialized halos.

Moving inward to the structure of stellar and galactic systems, we first looked at spherical systems. Specifically, we presented the singular isothermal sphere, a minimal starting model for a dark matter halo. We then moved on to systems with approximate cylindrical symmetry, studying thin disks and their perturbations. We showed how wave solutions are obtained that correspond to multiple spiral arms, helping to explain that most spectacular property of the images of galaxies. Finally, we introduced gravitational lensing, a beautiful consequence of general relativity that has many uses in astrophysics and cosmology.

We hope that the reader has noticed some common mathematical and physical threads at work throughout these chapters. The continuity, Euler, and Poisson equations were the basis of the analysis of cosmological linear perturbation theory in Chap. 4, stellar systems in Chap. 6, and galactic disks in Chap. 7. A linear analysis was performed both for cosmological perturbations and for spiral density waves. The mathematics of essentially Newtonian gravity was used to study cosmological spherical collapse (Sec. 5.1) and the two-dimensional problem of gravitational lensing (Sec. 8.3). The competition between random/dispersive velocities and

gravitationally-induced motions was the key to understanding both Jeans instability in the cosmological context (Sec. 4.5.5) and Toomre instability in galactic disks (Sec. 7.4.3).

The material in part I brings the reader up to a level of knowledge that enables a dip into recent research in galaxy formation. Part II is an in-depth review of one branch of this research, namely the study of cosmic dawn: the first stars and galaxies and the quest to observe them via the 21-cm line of hydrogen.

Part II

Early Galaxies and 21-cm Cosmology

This part focuses on cosmology and galaxies at high redshift, covering basic theory and recent research results on galaxy formation at early times, the supersonic streaming velocity, and the cosmic milestones of early radiative feedback. These subjects are all brought together under 21-cm cosmology, which is presented in some detail. The topics discussed here are of great interest in current research, and the high levels of activity and intensity are expected to last. Note that while Part I of this volume naturally reflects this author's personal style and preferences, this is even more so in Part II, which covers many topics involving the author's own work.

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Chapter 10

Overview

10.1. Brief outline

Understanding the formation and evolution of the first stars and galaxies represents one of the most exciting frontiers in astronomy. Since the universe was filled with hydrogen atoms at early times, the most promising method for observing the epoch of the first stars is to use the prominent 21-cm spectral line of hydrogen. Current observational efforts are focused on the cosmic reionization era, but observations of the pre-reionization cosmic dawn are also beginning and promise exciting discoveries. While observationally unexplored, theoretical studies predict a rich variety of observational signatures from the astrophysics of the early galaxies that formed during cosmic dawn. As the first stars formed, their radiation (plus that from stellar remnants) produced feedback that radically affected both the intergalactic medium and the character of newly-forming stars. Lyman- α radiation from stars generated a strong 21-cm absorption signal, observation of which is currently the only feasible method of detecting the dominant population of galaxies at redshifts as early as $z \sim 25$. Another major player is cosmic heating; if due to soft X-rays, then it occurred fairly early ($z \sim 15$) and produced the strongest pre-reionization signal, while if it is due to hard X-rays, as now seems more likely, then it occurred later and may have dramatically affected the 21-cm sky even during reionization. In terms of analysis, much focus has gone to studying the angle-averaged power spectrum of 21-cm fluctuations, a rich dataset that can be used to reconstruct the astrophysical information of greatest interest. This does not, however, diminish the importance of finding additional probes that are complementary or amenable to a more model-independent analysis. Examples include the global (sky-averaged) 21-cm spectrum, and the line-of-sight anisotropy of the 21-cm power spectrum. Another striking feature may result from a recently recognized effect of a supersonic relative velocity between the dark matter and gas. This effect enhanced large-scale clustering and, if early 21-cm fluctuations were dominated by small galactic halos, it produced a prominent pattern on 100 Mpc scales. Work in this field, focused on understanding

the whole era of reionization and cosmic dawn with analytical models and numerical simulations, is likely to grow in intensity and importance, as the theoretical predictions are finally expected to confront 21-cm observations in the coming years.

10.2. Detailed introduction

Galaxies around us have been mapped systematically out to a redshift $z \sim 0.3$ by recent large surveys [1, 2]. The observed galaxy distribution shows a large-scale filament-dominated “cosmic web” pattern that is reproduced by cosmological numerical simulations [3]. This structure is well-understood theoretically [4] as arising from the distribution of the primordial density fluctuations, which drove hierarchical structure formation in the early universe. Recent observations have been pushing a new frontier of early cosmic epochs, with individual bright galaxies detected reliably from as early as $z = 11.1$ [5], which corresponds to $t \sim 400$ Myr after the Big Bang. However, it is thought that the bulk of the early stars formed in a large number of very small galactic units, which will be difficult to observe individually. In particular, high-resolution numerical simulations show that the truly earliest stars formed within $\sim 10^6 M_\odot$ dark matter halos [6, 7]. These simulations can only follow small cosmic volumes, and thus begin to form stars much later than in the real universe, but analytical methods show that the very first such stars within our light cone must have formed at $z \sim 65$ (age $t \sim 35$ Myr) [8, 9]. The theoretical understanding of galaxy formation as related to the earliest generations of stars and galaxies has been reviewed extensively (e.g. [10, 11]).

The best hope of observing the bulk population of early stars is via the cosmic radiation fields that they produced. The mean radiation level traces the cosmic star formation rate, while spatial fluctuations reflect the clustering of the underlying sources, and thus the masses of their host halos. In particular, the hyperfine spin-flip transition of neutral hydrogen (H I) at a wavelength of 21 cm (Fig. 10.1) is potentially the most promising probe of the gas and stars at early times. Observations of this line at a wavelength of $21 \times (1 + z)$ cm can be used to slice the universe as a function of redshift z (or, equivalently, distance along the line of sight), just like any atomic resonance line in combination with the cosmological redshift. Together with the other two dimensions (angular position on the sky), 21-cm cosmology can thus be used to obtain a three-dimensional map of the diffuse cosmic H I distribution [12], in the previously unexplored era of redshifts $\sim 7 - 200$.

Absorption or emission by the gas along a given line of sight changes the 21-cm brightness temperature T_b , measured relative to the temperature of the background source, which here is the cosmic microwave background (CMB) [13]. The observed T_b is determined by the spin temperature T_S , an effective temperature that describes the relative abundance of hydrogen atoms in the excited hyperfine level compared to the ground state. Primordial density inhomogeneities imprinted a three-dimensional power spectrum of 21-cm intensity fluctuations on scales down to ~ 10 kpc (all sizes

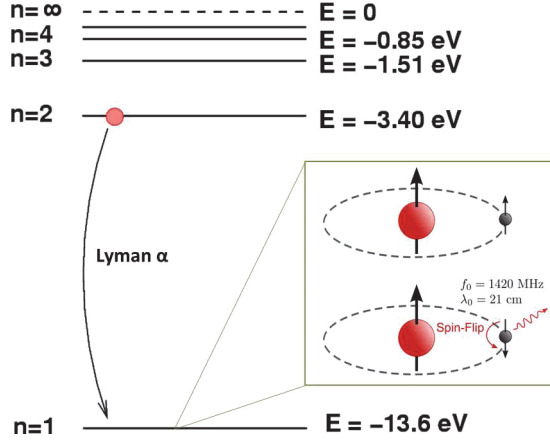


Fig. 10.1. The energy levels of hydrogen. The ionization energy of hydrogen is 13.6 eV, and the Lyman- α ($\text{Ly}\alpha$) line (10.2 eV) corresponds to the $n = 2$ to $n = 1$ transition. The spin-flip transition (inset on the right) is a much lower energy splitting (5.87×10^{-6} eV) within the ground state ($n = 1$) of hydrogen, corresponding to a wavelength of 21 cm and a frequency of 1420 MHz. Credits: Main portion: Michael Richmond (http://spiff.rit.edu/classes/phys301/lectures/spec_lines/spec_lines.html); Inset: Tiltec via Wikimedia Commons.

henceforth are comoving unless indicated otherwise), making it the richest dataset on the sky [14]. The potential yield of 21-cm observations is further increased by the expected anisotropy of the 21-cm power spectrum [15–18].

The 21-cm signal vanished at redshifts above $z \sim 200$, when the gas kinetic temperature, T_k , was close to the CMB temperature, T_{CMB} , making the gas invisible with respect to the CMB background. Subsequently, the gas cooled adiabatically, faster than the CMB, and atomic collisions kept the spin temperature T_S of the hyperfine level population below T_{CMB} , so that the gas appeared in 21-cm absorption [19]. As the Hubble expansion continued to rarefy the gas, radiative coupling of T_S to T_{CMB} started to dominate over collisional coupling of T_S to T_k and the 21-cm signal began to diminish.

Once stars began to form, their radiation produced feedback on the intergalactic medium (IGM) and on other newly-forming stars, and substantially affected the 21-cm radiation. The first feedback came from the ultraviolet (UV) photons produced by stars between the $\text{Ly}\alpha$ and Lyman limit wavelengths (i.e. energies in the range of 10.2 – 13.6 eV). These photons propagated freely through the Universe and some of them redshifted or scattered into the $\text{Ly}\alpha$ resonance, and coupled T_S to T_k once again [13] through the Wouthuysen-Field [20, 21] effect by which the two hyperfine states are mixed through the absorption and re-emission of a $\text{Ly}\alpha$ photon. Meanwhile, Lyman-Werner (LW) photons in nearly the same energy range (11.2 – 13.6 eV) dissociated molecular hydrogen and eventually ended the era of primordial star formation driven by molecular cooling [22], leading to the dominance of larger halos. X-ray photons also propagated far from the emitting sources and began

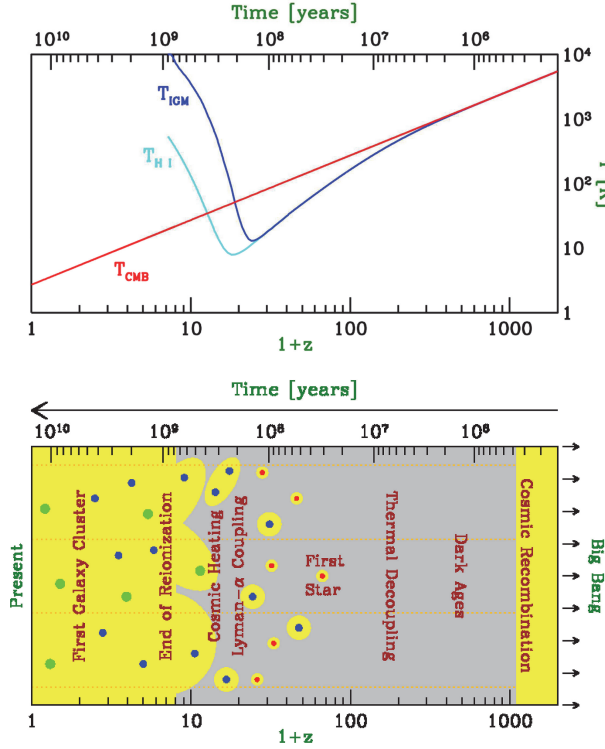


Fig. 10.2. Overview of cosmic history, with the age of the universe shown on the top axis and the corresponding redshift (plus one) on the bottom axis. Bottom panel: Yellow represents ionized hydrogen, and gray is neutral. Observers probe the cosmic gas using the absorption of background light (dotted lines) by atomic hydrogen. Stars formed in halos whose typical size continually grew with time, going from the first generation that formed through molecular-hydrogen cooling (red dots), to the larger galaxies that formed through atomic cooling and likely dominated cosmic reionization (blue dots), all the way to galaxies as massive as the Milky Way (green dots). Top panel: Corresponding sketch of the cosmic mean gas temperature within the IGM, including neutral regions only (cyan) or also ionized regions (blue) assumed to be at 10,000 K; these are compared to the CMB temperature (red curve). The gas was initially thermally coupled to the CMB, until it adiabatically cooled more rapidly, and was then heated first by X-ray heating and subsequently by reionization. Updated and expanded version of a Figure from [23].

early on to heat the gas [13]. Once T_S grew larger than T_{CMB} , the gas appeared in 21-cm emission over the CMB level. Emission of UV photons above the Lyman limit by the same galaxies initiated the process of cosmic reionization, creating ionized bubbles in the neutral gas around these galaxies. Figure 10.2 shows a brief summary of early cosmic history, and Table 10.1 lists the observed frequency corresponding to 21-cm radiation from various redshifts, as well as the age of the Universe.

The subject of cosmic reionization began in earnest after Gunn & Peterson (1965) [24] used a just-identified redshift $z \sim 2$ quasar to show that the Universe around it was highly ionized. This led to much theoretical work on how the Universe might have been reionized. The subject of 21-cm cosmology is a more recent

Table 10.1. The observed frequency corresponding to 21-cm radiation from a source at redshift z , and the age of the Universe, listed versus $1+z$. Units are as in the column labels except where indicated otherwise.

$1+z$	Observed 21-cm Frequency [MHz]	Cosmic Age [Myr]
1	1.42 GHz	13.8 Gyr
2	710	5.88 Gyr
3	473	3.29 Gyr
4	355	2.15 Gyr
7	203	934
10	142	547
15	94.7	297
20	71.0	192
25	56.8	137
30	47.3	104
40	35.5	67.5
50	28.4	48.2
60	23.7	36.5

one. Hogan & Rees (1979) [12] worked out the basic ideas and noted that 21-cm observations could probe the properties of cosmic gas including its density, temperature, and spin temperature (which, they noted, could be different from the kinetic temperature). Scott & Rees (1990) [19] revisited the subject, now in the modern context of galaxy formation in a Universe dominated by cold dark matter; they were the first to note that 21-cm cosmology could probe reionization. Madau *et al.* (1997) [13] first considered 21-cm radiation during cosmic dawn, before the epoch of reionization (EOR),¹ and highlighted the eras of Ly α coupling and of early cosmic heating. However, 21-cm cosmology was relatively slow in developing. For example, in a major review of the field in 2001 [10], we devoted 3 pages out of 114 to this topic, which at the time was considered only one of many promising avenues in the field.

Cosmic reionization remained the dominant subject in the field of the first stars for some time longer. After several years of confusion about the basic character of reionization (see Sec. 14.1), the now-standard paradigm was developed. Barkana & Loeb (2004) [25] showed that the surprisingly strong clustering of high-redshift halos leads to large ionized bubbles due to groups of clustered galaxies, and to an inside-out topology (with high-density regions reionizing early, leaving the voids for last). Furlanetto *et al.* (2004) [26] created a quantitative analytical model that yielded the first predictions of the distribution of H II bubble sizes, showing that 10 Mpc (comoving) is typical for the central stage of reionization. This picture

¹Two notes on common usage: The era/epoch of reionization is often denoted “EOR” in the literature; “Cosmic dawn” usually refers to the period between the formation of the first stars until the beginning of the EOR, although sometimes it is used as a general name for the entire period including the EOR.

of reionization based on semi-analytic models [25, 26] was then verified by large-scale numerical simulations, starting with Iliev *et al.* (2006) [27]. The theoretical expectation that the bubbles of reionization were large provides a critical boost for observational efforts to discover the resulting 21-cm fluctuations, since if higher angular resolution were required, this would make it harder to reach the sensitivity needed to detect the faint cosmic signal.

Cosmic reionization was initially thought to be the only source of fluctuations available for 21-cm interferometers (other than primordial density and temperature fluctuations, which create significantly smaller signals than those driven by galaxies and their strongly enhanced clustering). The earlier 21-cm events of cosmic dawn pointed out by Madau *et al.* (1997) [13] were considered to be highly uniform, since the photons that drove them ($\text{Ly}\alpha$ photons in the case of $\text{Ly}\alpha$ coupling, and X-ray photons in the case of cosmic heating) can travel ~ 100 Mpc in a neutral Universe before interacting. Unless rare objects such as quasars dominated, this seemed to imply a uniform cosmic transition that could only be seen with global 21-cm measurements that track the sky-averaged spectrum [28]. Cosmic dawn was opened up to interferometric observations when Barkana & Loeb (2005) [29] applied the same idea of unusually large fluctuations in the abundance of early galaxies, which had helped understand reionization, to earlier epochs. Spatial fluctuations in the $\text{Ly}\alpha$ intensity were shown to have led, in fact, to rather large 21-cm fluctuations from the $\text{Ly}\alpha$ coupling era. The same idea was then applied by Pritchard & Furlanetto (2007) [30] to the X-ray background during the cosmic heating era, showing that a large signal of 21-cm fluctuations should be expected in this case as well.

The entire story of 21-cm cosmology as described thus far is at the moment purely theoretical, but a great international effort is underway to open up the observational field of 21-cm cosmology. In particular, several arrays of low-frequency radio telescopes have been constructed (and are now operating) in order to detect the 21-cm fluctuations from cosmic reionization (and beyond). Current efforts include the Murchison Wide-field Array (MWA [31]), the Low Frequency Array (LOFAR [32]), the Giant Metrewave Radio Telescope (GMRT [33]), and the Precision Array to Probe the Epoch of Reionization (PAPER [34]), and future plans have been made for the Hydrogen Epoch of Reionization Array (HERA; <http://reionization.org/>) and the Square Kilometer Array (SKA; <https://www.skatelescope.org/>); a 21-cm cosmology pathfinder of the latter is the New Extension in Nançay Upgrading LOFAR (NenuFAR). Although the expected foregrounds (dominated by Galactic synchrotron) are much brighter than the 21-cm signal, they are not expected to include sharp spectral features. Thus, although ongoing experiments are expected to yield noisy maps, the prospects for extraction of the 21-cm signal (and from it the reionization history) are quite promising, using the key statistic of the 21-cm power spectrum [35–37] as well as other statistics [38–41]. A different approach is to measure the total sky spectrum and detect the global reionization signal arising from the overall disappearance of atomic hydrogen [42–44]; current and future efforts

(some also targeting eras before reionization) include the Experiment to Detect the Global EOR Step (EDGES [45]), the Large Aperture Experiment to Detect the Dark Ages (LEDA; <http://www.cfa.harvard.edu/LEDA/>), and the lunar-orbiting Dark Ages Radio Explorer (DARE; <http://lunar.colorado.edu/dare/>).

A novel effect that was only noticed fairly recently is the supersonic velocity difference between the gas and the dark matter [46]. This intriguing effect (often called the streaming velocity) is predicted to have influenced the gas distribution at high redshift as well as early galactic halos.

The plan for this part is to first build on the theoretical groundwork for galaxy formation presented in Part I with some additional topics focused on high-redshift galaxies. This is followed by the basics of 21-cm cosmology. Next comes a detailed discussion of the velocity streaming effect and its consequences. We then discuss in detail the milestones of radiative feedback during early cosmic history, and follow this with an outline of their 21-cm signatures. Finally, we summarize part II and conclude with a general outlook on the field.

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Chapter 11

Galaxy Formation: High-redshift Highlights

In this chapter we expand on several features of galaxy formation that are particularly important at high redshifts. We first briefly summarize a number of topics related to halos and the baryons within them. We then discuss fluctuations in the number density of galaxies, which are generally important in cosmology, but at high redshift the fluctuations become unusually large and this has significant consequences that reverberate throughout the remaining chapters of this work. Next, we discuss various challenges of numerical simulations and approaches to deal with them. While simulations have become an indispensable tool in cosmology, it is important to bear in mind that they have fundamental limitations, some of them specific to, or worsening at, high redshifts. For example, while simulations at low redshift can be continually tested by and improved based on astronomical observations, this is not currently possible (or is at least far more limited) at high redshift. Finally, we discuss the formation of the very first stars, obviously a subject of great theoretical and numerical interest, and with significant observational traces as well.

11.1. Halos and their gas content

11.1.1. *Halos: profiles and biased clustering*

Although spherical collapse (Sec. 5.1) captures some of the physics governing the formation of halos, structure formation in cold dark matter models proceeds hierarchically (Sec. 5.2). At early times, most of the dark matter is in low-mass halos, and these halos continuously accrete and merge to form high-mass halos. Numerical simulations of hierarchical halo formation indicate a roughly universal spherically-averaged density profile for the resulting halos (Navarro, Frenk, & White 1997 [1], hereafter NFW), though with considerable scatter among different halos. The NFW

profile has the form

$$\rho(r) \propto \frac{1}{c_N x (1 + c_N x)^2}, \quad (11.1)$$

where $x = r/r_{\text{vir}}$ and c_N is the concentration parameter. The logarithmic slope of this profile goes from -1 at small scales to -3 on large scales, with intermediate scales having a slope of -2 as in a singular isothermal sphere Sec. 6.6.2.

A key question in cosmology and galaxy formation is the spatial distribution of the halo number density. Since halos form due to gravity, massive halos should form in larger numbers in regions of high overall density than in low-density voids (see Sec. 3.4.3). Thus, density fluctuations are expected to lead to spatial fluctuations in the halo number density. This leads to the concept of halo (or galaxy) bias, a now-standard concept in galaxy formation [2–7]. Particularly simple is the case of linear bias, i.e. when the distribution of galaxies is a proportionally amplified (“biased”) version of that of the underlying density of matter. Mathematically this means that the relative fluctuations in the number density of galactic halos (δ_g) are proportional to the relative fluctuations in the underlying density of matter δ :

$$\delta_g = b \delta, \quad (11.2)$$

where b is the linear bias factor (or simply “the bias”).

This simple result is expected to be reasonably accurate when looking at fluctuations on large scales s (usually tens of comoving Mpc or more). Several conditions must be satisfied for this to be true. The scale s must be much larger than the spatial scales involved in forming the individual galactic halos whose clustering is being considered; this allows a separation of scales that is the basis of a simple approximation called a peak-background split [5]. Also, in order to avoid non-linear effects, the scale s must be large enough that typically $\delta \ll 1$, i.e. the variance is small when the density field is averaged on the scale s . Similarly, $\delta_g \ll 1$ on that scale is advisable. Finally, gravity must dominate galaxy formation, or at least, any other effects (such as astrophysical feedbacks) must operate on much smaller scales than s . Of these conditions, the first two tend to be more favorable at high redshifts, since the galaxies are typically small and thus associated with small formation scales, and density fluctuations on large scales are still relatively small. However, the last two conditions become more problematic, as discussed in great detail in the rest of part II. High-redshift galaxies are highly biased, so their fluctuations are much larger than those in the underlying density (Sec. 11.2); and since early galaxies were typically small, they were susceptible to a variety of external feedbacks that operate on scales of order 100 Mpc, including the supersonic streaming velocity (Chap. 13) and various radiative feedbacks (Chap. 14).

11.1.2. *Baryons: linear evolution, pressure, and cooling*

Baryons play a major role in cosmology. On the largest scales, their coupling to the photons in the early universe leaves them clustered differently from the dark matter,

with the difference decaying away only gradually. On smaller scales, the baryonic pressure suppresses gravitational growth. Most directly, of course, the baryons are important since stars form out of baryons that cool and collapse to high density.

As noted in Sec. 4.5.1, in the presence of dark matter only, the linear perturbations are dominated by a growing mode that is $\propto a$ in EdS, as the decaying mode drops rapidly, $\propto a^{-3/2}$ in EdS. On large scales, baryons also respond to gravity only (after cosmic recombination), but their initial conditions are different, as their strong coupling to the CMB photons up to recombination suppresses their sub-horizon fluctuations. Thus, cosmic recombination begins a period of baryonic infall, during which the baryons gradually catch up with the dark matter perturbations [8]. Specifically, if we denote the perturbations of the dark matter and baryon density δ_{dm} and δ_{b} , respectively, and their mass fractions within the total matter density $f_{\text{dm}} = (\Omega_{\text{m}} - \Omega_{\text{b}})/\Omega_{\text{m}}$ and $f_{\text{b}} = \Omega_{\text{b}}/\Omega_{\text{m}}$, then it is useful to work with the perturbation of the total density, δ_{tot} , and with the difference δ_{diff} , where

$$\delta_{\text{tot}} = f_{\text{dm}}\delta_{\text{dm}} + f_{\text{b}}\delta_{\text{b}}, \quad \delta_{\text{diff}} = \delta_{\text{b}} - \delta_{\text{tot}}. \quad (11.3)$$

In linear perturbation theory, δ_{tot} has the usual growing and decaying modes (i.e. $\propto a$ and $\propto a^{-3/2}$ in EdS), while the two solutions for δ_{diff} are constant ($\propto 1$) and $\propto a^{-1/2}$ in EdS. Thus, the baryon perturbation δ_{b} approaches δ_{tot} gradually from below. The rate of this approach can be described through their relative difference. If we approximately include only the dominant modes, this key quantity decays as [9]

$$r_{\text{LSS}} \equiv \frac{\delta_{\text{diff}}}{\delta_{\text{tot}}} \approx -\frac{0.3\%}{a}. \quad (11.4)$$

This decay is slow enough that the gradual baryonic infall is in principle observable in high-redshift 21-cm measurements [10] and perhaps also in the distribution of galaxies at low redshift [11, 12].

During this era of baryonic infall, and before cosmic heating from radiative astrophysical sources, the gas cooled adiabatically with the expansion. Traditional calculations [8, 13, 14] assumed a uniform speed of sound for the gas at each redshift, but a more careful consideration of the combination of adiabatic cooling and Compton heating substantially modifies the temperature perturbations on all scales [10, 15–17].

On small scales, the density evolution is no longer purely gravitational, as the gas pressure suppresses baryon perturbations. The relative force balance at a given time can be characterized by the Jeans scale (Sec. 4.5.5). If the gas has a uniform sound speed then the comoving Jeans wavenumber k_{J} is given by Eq. (4.63). In the simple limit where the gas cools adiabatically (after thermally decoupling from the CMB at $z \sim 140$), this gives a characteristic Jeans mass [based on Eq. (4.104)]

together with Eq. (4.102)] of [18]

$$M_J \equiv \frac{4\pi}{3} \left(\frac{\pi}{k_J} \right)^3 \bar{\rho}_m = 5.89 \times 10^3 \left(\frac{\Omega_m h^2}{0.141} \right)^{-1/2} \left(\frac{\Omega_b h^2}{0.0221} \right)^{-3/5} \left(\frac{1+z}{10} \right)^{3/2} M_\odot. \quad (11.5)$$

The Jeans mass, however, is not the whole story, since it is related only to the evolution of perturbations at a given time. When the Jeans mass itself varies with time, the overall suppression of the growth of perturbations depends on a time-averaged Jeans mass, the filtering mass [19]. To define it, we start from the regime of large-scale structure (i.e. scales too large to be affected by pressure, but much smaller than the horizon and the scale of baryon acoustic oscillations), where, as noted above, r_{LSS} does not depend on k , and is simply a function of redshift. On smaller scales, the next-order term describing the difference between the baryons and dark matter is the k^2 term [19], and the filtering wavenumber k_F and corresponding mass scale M_F are defined through [9]

$$\frac{\delta_b}{\delta_{\text{tot}}} = 1 + r_{\text{LSS}} - \frac{k^2}{k_F^2}; \quad M_F \equiv \frac{4\pi}{3} \left(\frac{\pi}{k_F} \right)^3 \bar{\rho}_m. \quad (11.6)$$

This filtering mass scale captures how the whole history of the evolving Jeans mass affects the final baryon perturbations that result at a given time. Starting at early times, since the baryon fluctuations are very small before cosmic recombination, the gas pressure (which depends on δ_b) starts out small, so the filtering mass starts from low values and rises with time up to a value of $\sim 3 \times 10^4 M_\odot$ [9] around redshift 30. It then drops due to the cooling cosmic gas, but the drop is very gradual (reaching $\sim 2 \times 10^4 M_\odot$ at $z = 10$ in the absence of cosmic heating or reionization) due to the remaining after-effects of the suppression of gas infall at higher redshifts. This behavior is significantly different from the Jeans mass, which declines rapidly with time [see Eq. (11.5)] and drops below $10^4 M_\odot$ at $z \simeq 13$.

What makes the filtering mass even more useful is that it seems to offer in many situations a good estimate of the minimum halo mass that manages to accrete a significant amount of gas (e.g. 50% of the cosmic baryon fraction). It is natural to expect some relation between this characteristic, minimum halo mass and the filtering mass, since the gas fraction in a collapsing halo reflects the total amount of gas that was able to accumulate in the collapsing region during the entire, extended collapse process. For example, a sudden change in gas temperature immediately begins to affect gas motions (through the pressure-gradient force), but has only a gradual, time-integrated effect on the overall amount of gas in a given region. In this way, the minimum accreting mass is analogous to the linear-theory filtering mass. However, the former is defined within the deeply non-linear regime, so the two masses may not necessarily agree quantitatively.

Gnedin [20] first compared the filtering mass to the characteristic mass in numerical simulations, suggesting that they are approximately equal in the post-reionization universe in which the IGM is hot and ionized. However, he used a

non-standard definition of the filtering mass that equals 8 times the standard definition given above. Subsequently, higher-resolution simulations did not find a clear relation between the theoretically calculated filtering mass and the characteristic mass measured in post-reionization simulations [21, 22]. However, the heating within simulations of inhomogeneous reionization is complex, and thus the filtering mass (which depends on the thermal history) is difficult to compute directly. The filtering mass has been shown to agree to within a factor of ~ 1.5 with the characteristic mass measured in simulations at higher redshifts, throughout the era prior to significant cosmic heating or reionization, as well as after a controlled, sudden heating [23, 24]. Thus, the issue of the possible usefulness of the filtering mass after reionization has not been settled, but alternative models have been recently proposed to fit results from post-reionization simulations [25, 26].

The conclusion is that prior to cosmic heating and reionization, gas is expected to accumulate significantly in dark matter minihalos down to a mass of $\sim 3 \times 10^4 M_\odot$ [24]. This minimum accretion mass later rises during cosmic heating and even more rapidly within ionized regions during cosmic reionization. In addition, even at the highest redshifts, the minimum mass is boosted in regions of significant streaming velocity (see Chap. 13 below).

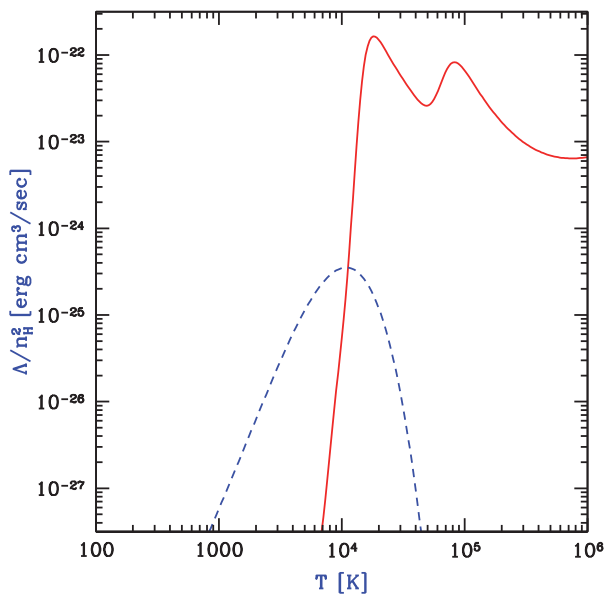


Fig. 11.1. Cooling rates as a function of temperature for a primordial gas composed of atomic hydrogen and helium, as well as molecular hydrogen, in the absence of any metals or external radiation. The plotted quantity Λ/n_H^2 is roughly independent of density (unless $n_H \gg 10 \text{ cm}^{-3}$), where Λ is the volume cooling rate (in erg/sec/cm^3). The solid line shows the cooling curve for an atomic gas, with the characteristic peaks due to collisional excitation of H I and He II. The dashed line shows the additional contribution of molecular cooling, assuming a molecular abundance equal to 0.1% of n_H . From [18].

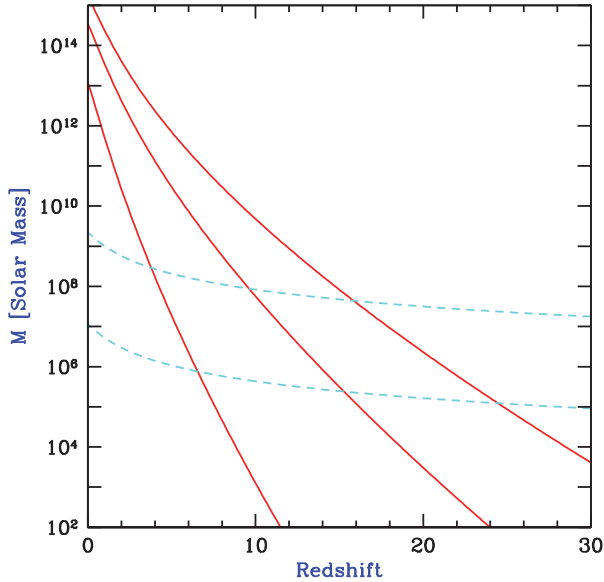


Fig. 11.2. Characteristic mass of galactic halos. The solid curves show the mass of collapsing halos that correspond to 1σ , 2σ , and 3σ fluctuations (in order from bottom to top). The dashed curves show the mass that approximately corresponds to the minimum temperature required for efficient cooling with primordial atomic species only (upper curve), or with the addition of molecular hydrogen (lower curve).

We end this section with a brief summary of cooling. Figure 11.1 shows the cooling curve for primordial gas, prior to metal enrichment. Primordial *atomic* gas can radiate energy only once hydrogen or helium are significantly ionized, so such cooling is limited to gas at temperatures above $\sim 10^4$ K. At high redshifts, most of the gas is in halos with relatively low masses, so that even if the accreted gas is shocked and heated to the virial temperature [Eq. (5.34)], it is unable to cool. However, in the presence of even a small ionized hydrogen fraction, molecular hydrogen can acquire sufficient abundance to provide significant cooling [27], and its rotational and vibrational transitions allow cooling down to below 10^3 K. The need to cool implies that stars at high redshift form in halos that correspond to rare density fluctuations (see Fig. 11.2). Further details about primordial gas cooling are reviewed elsewhere [18].

11.2. Large fluctuations in the galaxy number density

A broad, common thread runs through much of the recent theoretical development of cosmic reionization and 21-cm cosmology: The density of galaxies (or stars) varies spatially, with the fluctuations becoming surprisingly large at high redshift, even on quite large cosmological scales [28]. This can be understood from the standard

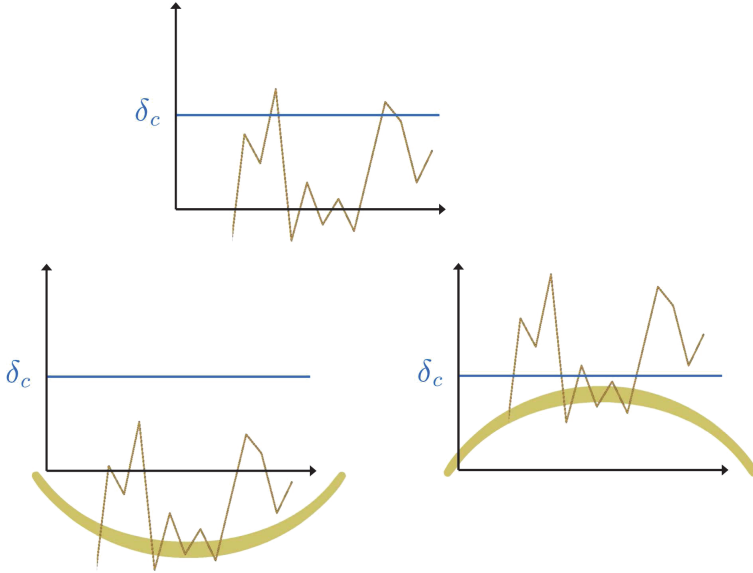


Fig. 11.3. Simple illustration of the large bias of high-redshift galaxies, which is the main idea driving the character of reionization [28] and the 21-cm fluctuations during cosmic dawn [29]. To form a halo, the total (linearly-extrapolated) density fluctuation must reach a value δ_c [denoted $\delta_{\text{crit}}(z)$ in Eq. (5.27)], from the sum of large-scale and small-scale density fluctuations. Thus, a large-scale void (bottom left) might have no halos, a typical region (top) a couple small halos, while a region with a large-scale overdensity (bottom right) will have many halos, both small and large. See text for additional explanation.

theory of galaxy formation as due to the fact that the first galaxies represented rare peaks in the cosmic density field.

As an analogy, imagine searching on Earth for mountain peaks above 5000 meters. The 200 such peaks are not at all distributed uniformly but instead are found in a few distinct clusters on top of large mountain ranges. Similarly, in order to find the early galaxies, one must first locate a region with a large-scale density enhancement, and then galaxies will be found there in abundance. For a more detailed argument, note that galactic halos form roughly in regions where the (linearly extrapolated) density perturbation reaches above a fixed threshold value $\delta_{\text{crit}}(z)$ (see Sec. 5.1.3). Now, the total density at a point is the sum of contributions from density fluctuations on various scales (Fig. 11.3). For initial perturbations from inflation (which follow the statistics of a Gaussian random field), the fluctuations on different scales are statistically independent. Thus, the same small-scale density fluctuations are added, in different regions, to various long-wavelength density fluctuations. In an over-dense region on large scales, the small-scale fluctuations only need to supply the missing amount needed to reach $\delta_{\text{crit}}(z)$, while in a large-scale void, the same small-scale fluctuations must supply a total density of $\delta_{\text{crit}}(z)$ plus the extra density missing within the void. This means that a larger fraction of the

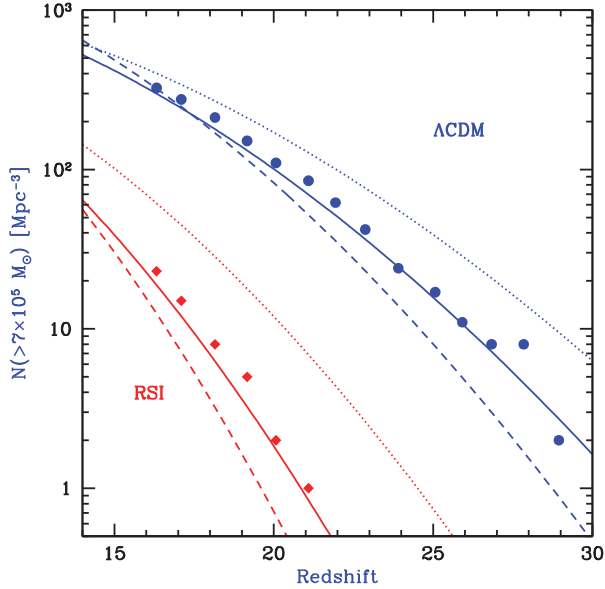


Fig. 11.4. Halo mass function at high redshift in a 1 Mpc box at the cosmic mean density. Data points show the number of halos above mass $7 \times 10^5 M_\odot$ as measured in simulations (from Figure 5 of [30]) with two different sets of cosmological parameters, the scale-invariant Λ CDM model of [30] (upper curves), and their running scalar index (RSI) model (lower curves). Each data set is compared with three theoretically predicted curves. The simulated values are well below the cosmic mean of the halo mass function (dotted lines). However, the prediction of the Barkana & Loeb (2004) [28] hybrid model (solid lines) takes into account the periodic boundary conditions of the small simulation box and matches the simulation results fairly well. The pure extended Press–Schechter model (dashed lines) is too low. From [28].

volume within the over-dense region will reach above $\delta_{\text{crit}}(z)$ in total density, and thus more halos will form there. Now, at high redshift, when density fluctuations had not yet had time for much gravitational growth, the effective threshold value $\delta_{\text{crit}}(z)$ is many times larger than the typical density fluctuation on the scales that form galactic halos. In other words, each halo represents a many- σ fluctuation. Under Gaussian statistics, the fraction of points above $t\sigma$ changes rapidly with t , once t is 2–3 or higher. Thus, the abundance of halos in a given region changes rapidly with small changes of the mean density in the region (and this mean density is set by large-scale density modes). The density of star formation is thus expected to show strongly biased (i.e. amplified) fluctuations on large scales [28]. These large-scale fluctuations at high redshift, and their great observational importance, had for a long time been underestimated, in part because the limited range of scales available to numerical simulations put these fluctuations mostly out of their reach.

Figure 11.4 illustrates a further effect, which is that the limited box size of simulations leads to a delay of halo formation, or equivalently, an underestimate of the abundance of halos (and stars) at any given time. The reason is that the periodic

boundary conditions within the finite simulation box artificially set the amplitude of large-scale modes (above the box size) to zero. There are many such volumes in the real Universe, with various mean densities (that follow a Gaussian distribution, within linear perturbation theory). Since galaxies (especially at high redshift) are highly biased, most of them form in those volumes that have an unusually high mean density. Thus, a simulated volume at the cosmic mean density is not representative of the locations of stars.

This limitation of simulations is most acute for the very first star in the Universe, a challenge of special interest for simulators because it represents in principle a perfectly clean problem, before the first entrance of the complexities of astrophysical feedback from prior star formation. The very first star formed in a very rare high-density region. Indeed, the large size of the real Universe allowed such a rare fluctuation to be found somewhere by chance, but it is unlikely to be found within a small simulation box, even if the simulation has the right abundance of galaxies (while real simulations, in addition, artificially lower this abundance when setting the mean density in the box to the cosmic mean density). For example, one of the first high-resolution “first star” simulations formed its first star only at redshift 18.2 [31], while analytical methods show that the first star is expected to have formed from an 8σ fluctuation at $z \sim 65$ [32, 33] within our past light cone (i.e. so that we can in principle see them as they formed), or a further $\Delta z \sim 6$ earlier [34] within the entire volume of the observable Universe (so that we can see them or their remnants after they formed). On this point, we note that there were some early, rough analytical estimates of the formation redshift of the very first stars [35, 36].

More generally, Barkana & Loeb (2004) [28] developed a hybrid model that allows one to predict the modified halo mass function in regions of various sizes and various average densities. As noted in section 5.4, for the cosmic mean halo abundance, the classic Press–Schechter [2] model works only roughly, while the halo mass function of Sheth & Tormen (1999) [37] (with modified best-fit parameters [38]) fits numerical simulations much more accurately [39]. Now, a generalization of the Press–Schechter model known as the extended Press–Schechter model [6] allows the prediction of the halo mass function in a given volume (of given size and mean density) compared to the cosmic mean mass function. No simple generalization of this type is known for the Sheth–Tormen mass function, but Barkana & Loeb [28] pointed out that this problem can be overcome since the prediction of the extended Press–Schechter model for the change *relative* to the cosmic mean mass function has been shown to provide a good fit to numerical simulations over a wide range of parameters [7, 38, 40]. Thus, the Barkana & Loeb [28] hybrid model starts with the Sheth–Tormen mass function and applies a correction based on the extended Press–Schechter model. The model gives a good match to simulations even in volumes that strongly deviate from the cosmic mean halo function (Fig. 11.4).

The idea of unusually large fluctuations in the abundance of early galaxies first made a major impact on studies of cosmic reionization, leading to the conclusion

that reionization occurs inside-out, with typical H II bubbles that are larger and thus easier to observe than previously thought [28] (see Sec. 14.1). The same idea soon found another important application in a different regime, leading to the prediction of 21-cm fluctuations from earlier times during cosmic dawn. The study of fluctuations in the intensity of early cosmic radiation fields began with Ly α radiation [29] (see Sec. 14.2) and continued to other fields including the X-rays responsible for early cosmic heating [41] (see Sec. 14.3). These are all sources of 21-cm fluctuations, and are thus the main targets for 21-cm radio interferometers. Clearly, the idea of substantial large-scale fluctuations in galaxy numbers is a driver of much of the current theoretical and observational interest in 21-cm cosmology as a way to probe the era of early galaxy formation. The recent discovery of the streaming velocity (see Chap. 13) has added a new flavor to this general theme.

11.3. Simulations at high redshift: challenges and approaches

In this section we discuss several aspects of simulations of the high-redshift Universe. First, we discuss some challenges and limitations of current numerical simulations, particularly when applied to early galaxy formation at high redshifts. Some of the issues we discuss can be addressed with additional study (e.g. setting the initial conditions accurately), while other difficulties are likely to remain for the foreseeable future (such as uncertainties related to star formation and stellar feedback). We then briefly discuss other approaches: analytical models and semi-numerical simulations.

We begin with a number of challenges that are important to recognize when evaluating the results of numerical simulations. As explained in the previous subsection, the large size of the real Universe implies that stars began to form very early. More generally, halos of various masses (or circular velocities) are predicted to have begun to form much earlier than the typical redshifts we are accustomed to, both from current numerical simulations and current observations. Figure 11.5 shows that while the very first star formed (in our past light cone) via molecular cooling at $z \sim 65$, the first generation of more massive atomic-cooling halos formed at $z \sim 47$ [32]. While the Milky Way halo mass is fairly typical in today's Universe, the very first such halo formed at $z \sim 11$, and the first Coma cluster halo at $z \sim 1.2$.

A direct simulation of the entire observable universe out to the spherical shell at redshift 70 would require a simulated box of length 25,000 Mpc on a side. Actual simulations, which often form a “first star” at redshift 20 or 30, effectively explore a very different environment from $z \sim 65$, in terms of the CMB temperature, the cosmic and virial halo densities (of both the dark matter and gas), the halo merger history, and high-redshift effects such as the difference between the power spectra of baryons and dark matter (discussed further below). Even if simulations do not attempt to approach the very first star, critical physical effects at high redshift push simulations towards the requirement of large boxes. The fact that the typical bubble scale of cosmic reionization is tens of Mpc (see Sec. 14.1) already implies

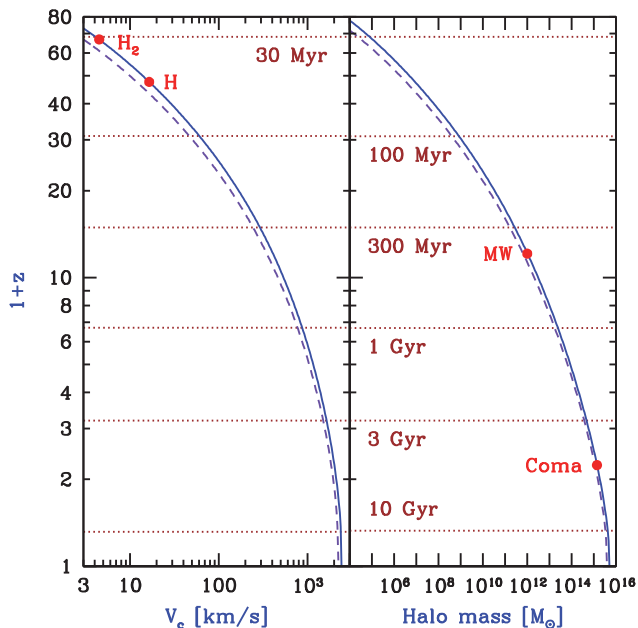


Fig. 11.5. The median redshift for the first appearance (in our past light cone) of various populations of halos: either halos above a minimum circular velocity (left panel) or a minimum mass (right panel). Dots indicate in particular the first star-forming halo in which H_2 allows the gas to cool, the first galaxy that forms via atomic cooling (H), as well as the first galaxy as massive as our own Milky Way and the first cluster as massive as Coma. The horizontal lines indicate the elapsed time since the Big Bang. The results from two sets of cosmological parameters (solid curves [42] and dashed curves [43]) illustrate the systematic error due to current uncertainties in the values of the cosmological parameters. From [32].

a minimum box size of ~ 100 Mpc for this era. However, the streaming velocity (Chap. 13), which is important early on, has a typical coherence scale of ~ 100 Mpc, and the radiation fields responsible for early feedback (Chap. 14) — $\text{Ly}\alpha$ coupling, Lyman–Werner feedback, and cosmic heating — fluctuate significantly on a similar scale. In particular, hard X-rays heat from afar and can extend the heating era into cosmic reionization (Sec. 14.3 and Sec. 15.4).

A significant presence of any one of these effects is enough to force any reasonable simulation during these epochs to a minimum box size of ~ 400 Mpc. Another consideration that pulls in the same direction is that observations of the 21-cm signal are easier (and currently only possible) on large scales. The sensitivity of a radio interferometer is degraded as the angular resolution is increased [Eq. (12.34)]. Thus, numerical simulations are squeezed between the need to cover a huge volume, on the one hand, and the need to adequately resolve each halo, on the other hand. This becomes especially demanding at early times, when most of the star formation occurs in very low-mass halos. Consider, for example, an N-body simulation of a 400 Mpc box in which $10^6 M_\odot$ halos are resolved into 500 dark matter particles each.

Extensive tests [44] show that this resolution is necessary in order to determine the overall properties of an individual halo (such as halo mass) just crudely, to within a factor of two; for better accuracy or to determine properties such as star formation, more particles are required. Even with just 500, this would require a simulation with a total of 10^{15} particles, much higher than numbers that are currently feasible. Truly resolving star formation within these halos would also require hydrodynamics and radiative transfer at much higher resolution still.

Naoz *et al.* (2006) [32] pointed out another limitation of current simulations, namely that they do not determine their initial conditions accurately enough for achieving precise results for high-redshift halos, especially those hosting the very first stars. Simulations assume Gaussian random initial fluctuations as might be generated by a period of cosmic inflation in the early Universe. The evolution of these fluctuations can be calculated exactly as long as they are small, with the linearized Einstein–Boltzmann equations. The need to begin the simulation when fluctuations are still linear forces numerical simulations of the first star-forming halos to start at very high redshifts (much higher than starting redshifts in common use that are often around $z = 200$). According to spherical collapse, a halo forming at redshift z_{form} has an extrapolated linear overdensity of $\delta = \delta_c \sim 1.7$ [Eq. (5.12)].

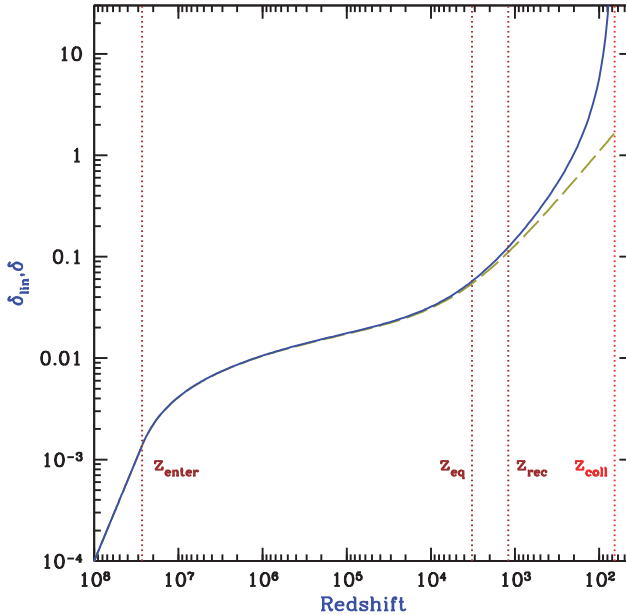


Fig. 11.6. Evolution of the fractional overdensity δ for a spherical region containing $10^5 M_\odot$ that collapses at $z = 66$ (approximately corresponding to the host halo of the very first star in our past light cone). We show the fully non-linear δ (solid curve) and the linearly-extrapolated δ (dashed curve). We indicate the redshifts of halo collapse (z_{coll}), cosmic recombination (z_{rec}), matter-radiation equality (z_{eq}), and entry into the horizon (z_{enter}). Note that the overdensity shown here corresponds to synchronous gauge [13], similarly to the analysis in Sec. 4.5.6. From [32].

Since it grows roughly with the EdS growing mode, the corresponding perturbation (in the dark matter) is $\delta \sim 13\% [(1 + z_{\text{form}})/66]$ at cosmic recombination, and $\delta \sim 6\% [(1 + z_{\text{form}})/66]$ at matter-radiation equality (see Fig. 11.6). The perturbation reaches $\delta \sim 1\% [(1 + z_{\text{form}})/66]$ extremely early, at $z \sim 10^6$. It re-enters the horizon (after having left during inflation) when $\delta \sim 0.2\% [(1 + z_{\text{form}})/66]$ at $z \sim 3 \times 10^7$; precision at this level would require setting initial conditions with a non-linear general relativistic calculation.

In addition to the problem of non-linearity, there is also the influence of early cosmic history on the linear and (more challengingly) non-linear initial conditions. Effects that must be taken into account include the contribution of the radiation to the cosmic expansion, suppression of sub-horizon perturbations in the photon density by the radiation pressure, and the coupling of the baryons to the photons which suppresses baryon perturbations until cosmic recombination. Within a spherical collapse calculation, Naoz *et al.* [9, 32] calculated halo formation including all these effects (Fig. 11.6), and found that they result in an earlier formation redshift for the first star by 3.3% in $1+z$ (compared to using the standard results from spherical collapse). The extended period at high redshift when the baryon perturbations remain suppressed compared to the dark matter is the main cause of this shift in the formation time, but the contribution of the photons to the expansion of the universe also makes a significant contribution. A 3.3% change in $1+z$ at $z \sim 65$ corresponds to a 4.8% change in the age of the universe, and to an order of magnitude change in the abundance of halos at a given redshift at $z \sim 65$. The shift in $1+z$ for the formation of a given halo goes down with time but is still 1% at $z \sim 20$. In addition, early cosmic history has a major impact (by factors of two or more) on the amount (and distribution) of gas that accumulates in the halos that hosted the first stars [24] (see the discussion of the filtering mass in Sec. 11.1.2); this effect is increased further by the presence of the streaming velocity (see Chap. 13), an effect that has been included in few first-star simulations. Therefore, even mild precision in numerical simulations of the formation of the first stars requires a calculation of these effects on halo formation, in combination with the above-mentioned issue of non-linearity going back to extremely early times.

Thus, while some processes are calculated with very high precision in numerical simulations, there are much larger effects that must be confronted before the results can be considered to accurately reflect the first stars in the Universe. Even in the limit of the very first stars, ostensibly a very clean problem for numerical simulations, the effects just discussed make the problem difficult, since many relevant physical processes must be included and numerical convergence must be fully demonstrated. The current status of numerical simulation results on the formation of the first stars is summarized below (Sec. 11.4).

Numerical simulations of galaxy formation *beyond* the very first star (in a given cosmological region) face even bigger problems, which can be summarized with one word: feedback. Long-distance feedback directly from stellar radiation is

generated by Ly α photons (reaching out to ~ 300 Mpc), Lyman–Werner photons (out to ~ 100 Mpc), and UV ionizing photons (initially absorbed in the immediate surroundings, but reaching up to ~ 70 Mpc by the end of reionization [45]). Some stars have strong stellar winds, and some explode in supernovae, which deposit thermal and kinetic energy as well as metals. Stellar remnants such as X-ray binaries produce X-rays which include hard photons that reach cosmological distances. Central black holes may also produce thermal and kinetic feedback, as well as UV and X-ray radiation. Most types of radiation that are responsible for feedback can be partially absorbed or scattered within the emitting galaxy or its immediate surroundings, another important process that depends on the detailed, small-scale distribution of gas and metals. Given the basic uncertainties about the detailed physics even of well-observed present-day astrophysical phenomena such as magnetic fields, dust, supernovae, the stellar initial mass function, and central black holes, ab-initio numerical simulations that are truly self-contained do not seem feasible. Once these various feedback effects begin to operate, they strongly affect the properties of subsequent generations of stars and galaxies, so that many observable predictions become strongly dependent on the generation and results of feedback. Numerical simulations can offer increasingly precise gravity, hydrodynamics, and radiative transfer, but are often limited by simplistic models of star formation and feedback that are inserted by hand. A major issue with astrophysical sources is that truly simulating their formation process, detailed structure, and feedback would require resolving length scales that are around 20 orders of magnitude smaller than the cosmological distances reached by some of the photons responsible for radiative feedback. The resulting vast gulf between the resolution of cosmological simulations and that of reality means that increasing resolution does not necessarily imply convergence towards the correct final answer; there could be multiple regimes of apparent convergence as additional levels of resolution uncover new physical processes.

On the opposite end from simulations are analytical (or semi-analytical) models. These models are very flexible, can be easily used to explore a wide variety of astrophysical possibilities and to incorporate a range of astrophysical uncertainties, and can be directly fit to data in order to determine the parameters of well-fit models. Such models can also be made more quantitatively accurate by basing them on fits to the results of numerical simulations of early galaxy formation. However, analytical models are also significantly limited. In 21-cm cosmology, perhaps their biggest limitation is that they usually must assume linear perturbations. While large-scale density fluctuations are indeed fairly small at early times, the large bias of high-redshift galaxies (Sec. 11.2) leads to quite non-linear fluctuations in the radiative, astrophysical sources of 21-cm fluctuations. In addition, the highly non-linear fluctuations on small scales do not completely average out when smoothing on large scales (as in real observations). This is due to additional non-linear relationships in 21-cm cosmology such as the dependence of 21-cm temperature on gas temperature

[Eq. (12.14) or Eq. (12.20)]. Thus, analytical calculations based on assuming linear perturbations and linear bias are quite limited in their accuracy (An important example is the discussion in Sec. 12.3 of non-linear limits on the accuracy of the linear result for the anisotropy of the 21-cm power spectrum).

The limitations of both numerical simulations and analytical models have led to the rise of an intermediate approach that combines some of the advantages of both. This method is termed hybrid, or semi-numerical simulation. While there are several specific approaches, the basic idea is to calculate physical processes directly on large scales, where everything is relatively simple, and indirectly on small, highly non-linear scales. On the small scales, halos and their properties are often adopted from semi-analytical models that have been fitted to numerical simulation results, or sometimes directly from the outputs of N-body (i.e. gravity-only) simulations plus some assumptions about star formation and other astrophysics. On the large scales, radiation such as X-rays, LW, and Ly α photons can be directly summed from all sources, albeit with a few approximations (e.g. the optical depth calculated assuming the cosmic mean density, and multiple scattering of Ly α photons treated approximately). Also, for reionization, such codes usually employ an approximation based on an analytical model for the distribution of H II bubble sizes [46] (Sec. 14.1); fortunately, the resulting ionized bubble distribution is quite similar to the results of radiative transfer, except in the fine (small-scale) details (see Fig. 15.1 in Sec. 14.1). A successful, publicly-available semi-numerical code in 21-cm cosmology is 21CMFAST [47]; results from this code and from the code developed by the author's group [48] are shown in Chap. 15.

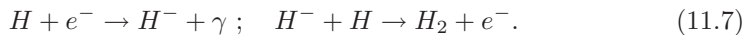
Summing up, numerical simulations of early galaxies offer the potential advantages of fully realistic source halo distributions and accurate gravity, hydrodynamics, and radiative transfer. However, much of the vitality of the field comes from the major uncertainties associated with the formation of, and feedback from, astrophysical sources. For example, it is possible that most early stars were much more massive and thus brighter than modern stars, or that a relatively large amount of gas collected within massive mini-quasars in the centers of galaxies. These astrophysical uncertainties will very likely be resolved only based on direct observational evidence. As we contemplate the range of possible observational predictions, it is much easier to explore a wide variety of astrophysical possibilities with simple analytical models or semi-numerical hybrid methods that combine processes on a large-scale grid with a sub-grid model based on numerical simulation results. Once the observations come in, there will be a need to fit astrophysical parameters to the data, and this requires a flexible framework and cannot be done directly with numerical simulations; once a well-fit model has been found, though, simulations may offer the best way to compare it in detail with the observations. It is important to note that discoveries in the field of the first stars and 21-cm cosmology (as summarized throughout part II) are often driven by large-scale processes, so due to the limited reach of simulations, many have come first from analytical or semi-numerical methods.

11.4. The very first stars

Numerical simulations are our best tool for trying to understand and predict the detailed properties of the first stars. It is important, though, to keep in mind the discussion in the previous two sections of the limitations of numerical simulations in general, and those of the first stars in particular. To summarize, the characteristics of first stars in simulations differ from true first stars in a number of ways: redshift ($z \sim 20-40$ compared to the true $z \sim 65$, which implies many important differences in the environment); rarity (the first stars correspond to statistical fluctuations that are much rarer than those in simulations, which gives them different characteristics); and initial conditions [the dark matter and, especially, baryonic density and velocity are affected by early cosmic history as well as by the streaming velocity, effects that are not accurately incorporated (if at all) in current numerical simulations].

The subject of first-star simulations has been extensively reviewed elsewhere [49, 50], but we briefly summarize it in this section. In principle, the formation of primordial stars is a clean numerical problem, as the initial conditions (including the distribution of the gas and dark matter and the chemical and thermal history of the gas) are cosmological and not yet affected by astrophysical feedback. One possible (though still speculative) complication is the generation and amplification of magnetic fields in the early universe in time for them to affect the formation of the first stars [49, 51–53].

As mentioned at the end of Sec. 11.1.2, under cosmological conditions, gas cooling in small early halos is possible only via molecular hydrogen cooling. Studies of the non-equilibrium chemistry of H_2 formation and destruction [54–58] concluded that H_2 formation in a collapsing small halo is dominated by the H^- channel, in which the residual free electrons from cosmic recombination act as catalysts:



Numerical simulation of the formation of a first (so-called Population III, or Pop III) star via H_2 cooling in a primordial minihalo of $10^5 - 10^6 M_\odot$ has proven to be a difficult problem, as initial results that established a prediction of single very massive stars have recently been replaced by a new paradigm of multiple stellar systems with a range of masses. Indeed, the first generation of simulations indicated the formation of massive Pop III stars of $\sim 100 M_\odot$. Such stars would be short-lived, generate extremely strong ionizing radiation and stellar winds, and end up producing massive black hole seeds or pair-instability supernovae. The expectation of massive stars was consistent between early simulations evolving an artificial overdensity with a smooth particle hydrodynamics (SPH) code (Fig. 11.7) and simulations that directly employed cosmological initial conditions along with the impressive resolution of an adaptive mesh refinement (AMR) code (Fig. 11.8).

Even for a given set of initial conditions for star formation, the final properties of the resulting stars depend on a complex process of proto-stellar evolution. It was

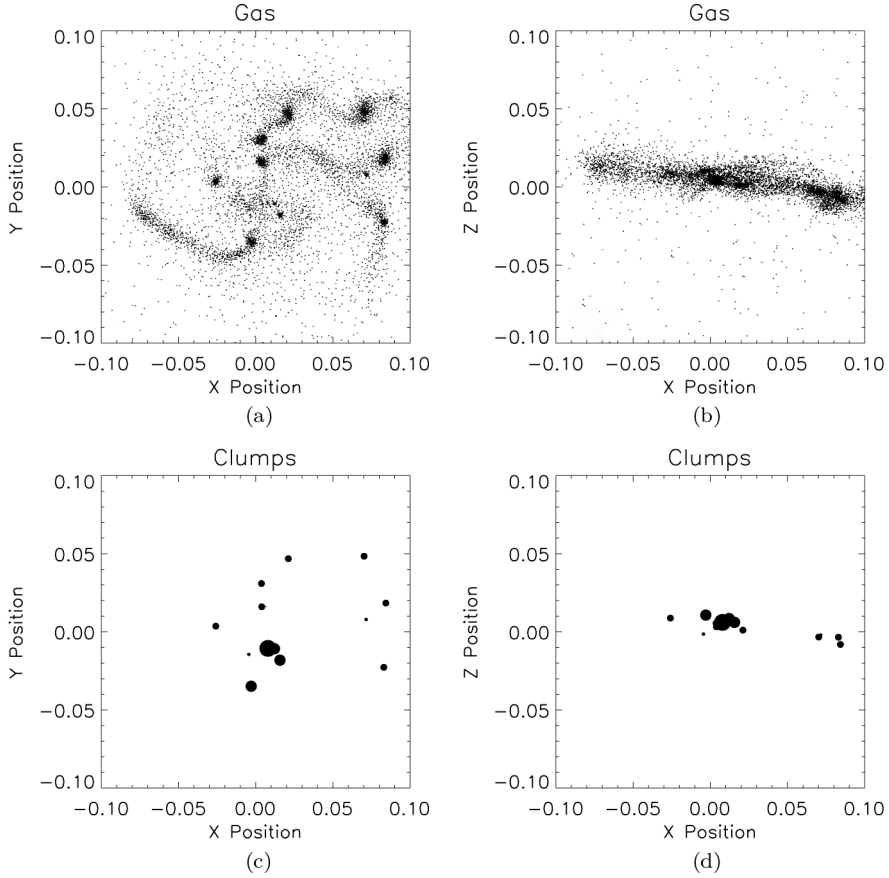


Fig. 11.7. Gas and clump morphology at $z = 28$ in the first-star simulation of Bromm *et al.* (1999) [59]. Top row: The remaining gas in the diffuse phase. Bottom row: The distribution of clumps, where the four increasing dot sizes denote increasing clump masses ($> 10^2 M_\odot$, $> 10^3 M_\odot$, $> 5 \times 10^3 M_\odot$, $> 10^4 M_\odot$). Left panels: Face-on view. Right panels: Edge-on view. The length of the box is 30 pc. The gas has settled into a flattened configuration with a number of dominant, massive clumps. From [59].

initially thought that the rapid accretion rates characteristic of primordial star-forming regions at high-redshift would naturally lead to isolated Pop III stars of $100 M_\odot$ or more. However, some simulations [60] then showed the possible formation of binaries (Fig. 11.9), and further semi-analytical and numerical simulation studies [61–66] have found that the clumps have sufficient angular momentum to form a disk, and that the rapid accretion onto the disk causes it to fragment due to gravitational instability. While it is too early to draw final conclusions, the best bet currently is that Pop III stars formed with a wide range of different masses, but on average were significantly heavier than later generations of stars (Fig. 11.10).

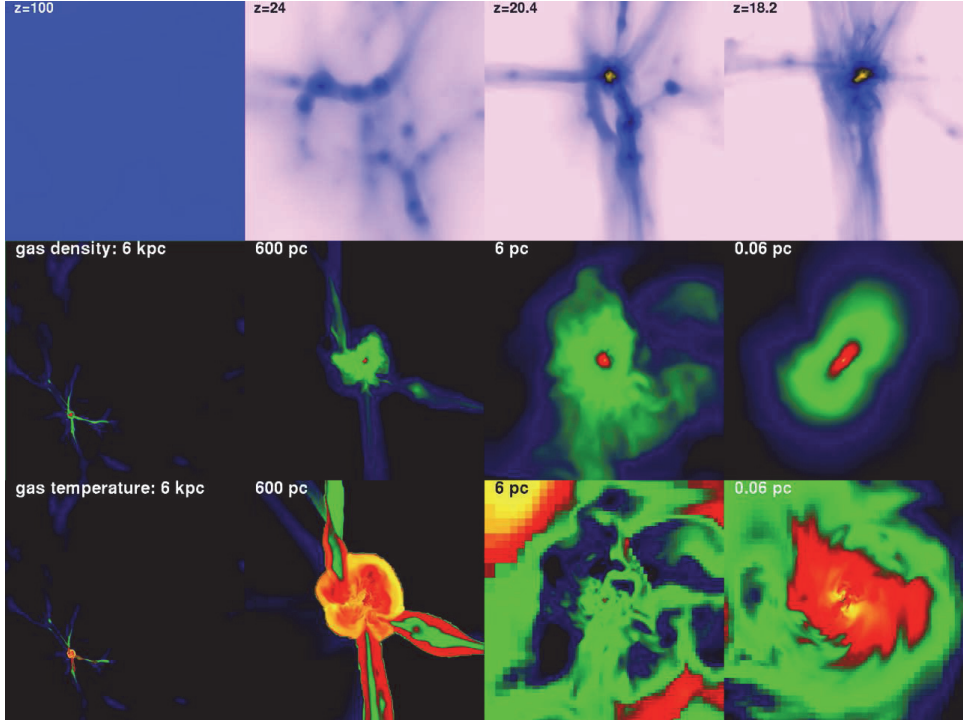


Fig. 11.8. The first star in a simulation by Abel *et al.* (2002) [31]. Top row: Projection of gas density on a 600 pc scale (all distances are physical in this Figure), at several redshifts. Other two rows: Slices of gas density or temperature on several different scales, all at the final redshift of the simulation ($z = 18.2$). From left to right, the two bottom rows show: large-scale filaments; the virial accretion shock; the H_2 cooled, high-redshift molecular cloud analog; and a warm core containing $\sim 100 M_\odot$ of gas. From [31].

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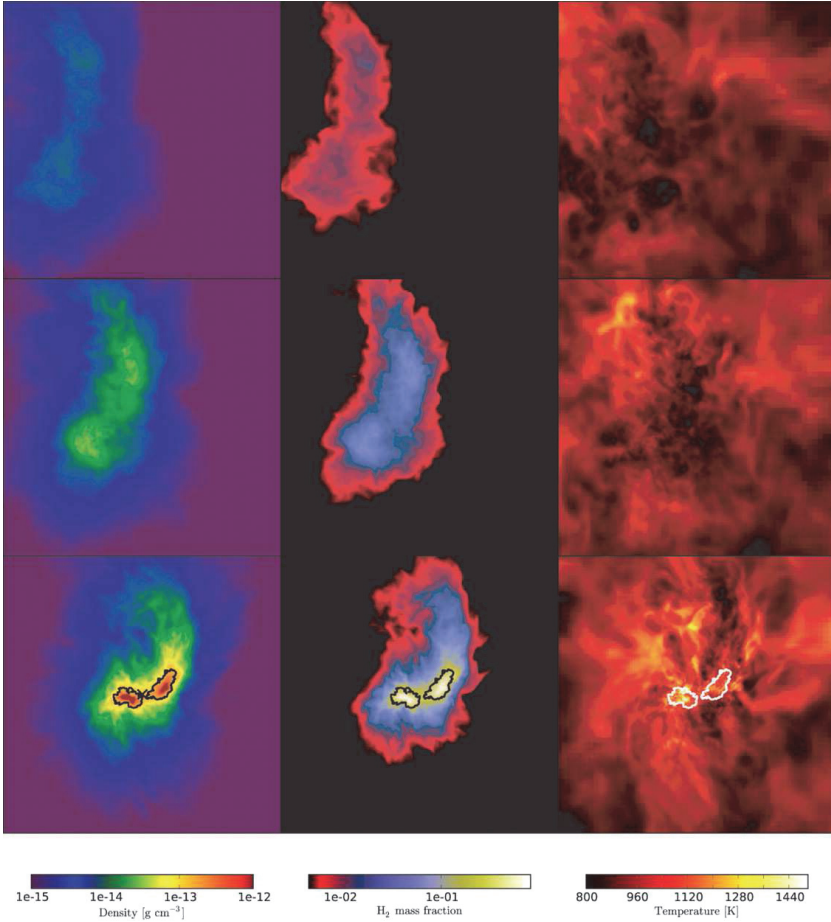


Fig. 11.9. The first stars may have been binaries, according to a simulation by Turk *et al.* (2009) [60]. Shown is the average density (left column), H_2 mass fraction (middle), and temperature (right), projected through a cube 3500 AU on a side. The bottom row (in which the two separate gravitationally-bound cores are outlined with thick lines) is at the end of the simulation, with the other rows showing earlier times by 555 years (middle) or 1146 years (top). From [60].

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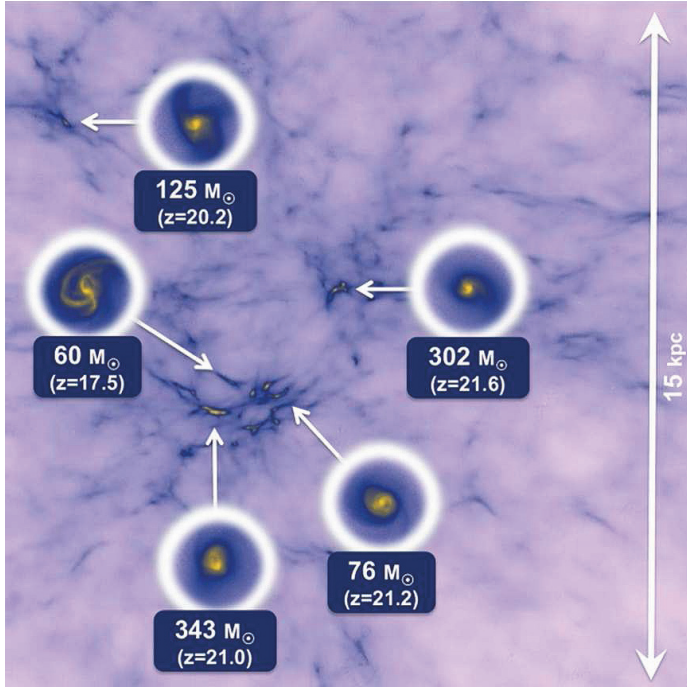


Fig. 11.10. The first stars may have had a range of masses, based on a simulation by Hirano *et al.* (2014) [65]. The projected gas density is shown at $z = 25$. Five primordial star-forming clouds are highlighted, with each circle showing a zoom-in to the central parsec at the formation time of the star; its formation redshift and stellar mass are listed. From [65].

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Chapter 12

21-cm Cosmology

An overview of the basic features and early development of 21-cm cosmology was given in Chap. 10. In this section we present the basic physics in greater detail, then focus on some important low-temperature corrections, and discuss the important subject of anisotropy in the 21-cm signal. Finally, we give a brief overview of the observational aspects of 21-cm cosmology, focusing on the power spectrum. More details of 21-cm physics and observational techniques are available in specific reviews of 21-cm cosmology [1–3].

12.1. Basic physics

The basic physics of the hydrogen spin transition is determined as follows. At the low densities typical in cosmological applications, the gas is far from full thermal equilibrium, and a single temperature cannot accurately describe the occupancy of various atomic levels. In particular, the relative occupancy of the spin levels is usually described in terms of the hydrogen spin temperature T_S , which is an effective temperature that determines the emission or absorption properties of the 21-cm line. Specifically, T_S is defined by

$$\frac{n_1}{n_0} = 3 \exp \left\{ -\frac{T_\star}{T_S} \right\}, \quad (12.1)$$

where n_0 and n_1 are the number densities of the singlet and triplet hyperfine levels in the atomic ground state ($n = 1$), respectively, and $T_\star = 0.0682$ K is defined by $k_B T_\star = E_{21}$, where the energy of the 21-cm transition is $E_{21} = 5.87 \times 10^{-6}$ eV, corresponding to a frequency of 1420 MHz (and a precise wavelength of $\lambda_{21} = 21.1$ cm). The factor of 3 in Eq. (12.1) is the ratio of statistical weights, i.e. it arises from the degeneracy factor of the spin 1 excited state. In particular, $T_S \rightarrow \infty$ would correspond to having the singlet and triplet levels populated in their statistical 1:3 ratio, $T_S \rightarrow 0$ would mean an empty excited state, while a population inversion (not expected in the cosmological 21-cm field) would correspond to negative T_S . Since

T_* is such a low temperature, in what follows we make the standard assumption that all other temperatures (including T_S) are much higher.

A patch of neutral hydrogen at the mean density and with a uniform T_S produces an optical depth at 21 cm [observed at $21(1+z)$ cm] of

$$\tau(z) = \frac{3c\lambda_{21}^2 h_P A_{10} n_{HI}}{32\pi k_B T_S (1+z) (dv_r/dr)}, \quad (12.2)$$

where h_P is Planck's constant, $A_{10} = 2.85 \times 10^{-15} \text{ s}^{-1}$ is the spontaneous decay rate of the hyperfine transition, n_{HI} is the number density of hydrogen atoms, and dv_r/dr is the gradient of the radial velocity along the line of sight, with v_r being the physical radial velocity and r the comoving distance. In a fully-neutral, homogeneous universe, $n_{HI} = \bar{n}_H(z)$ and $dv_r/dr = H(z)/(1+z)$ in terms of the Hubble parameter H . Assuming the high-redshift (EdS) form for $H(z)$ (see Sec. 2), this yields

$$\tau(z) = 9.85 \times 10^{-3} \left(\frac{T_{\text{CMB}}}{T_S} \right) \left(\frac{\Omega_b h}{0.0327} \right) \left(\frac{\Omega_m}{0.307} \right)^{-1/2} \left(\frac{1+z}{10} \right)^{1/2}, \quad (12.3)$$

where T_S and T_{CMB} are measured at z . Since the brightness temperature through the IGM is $T_b^z = T_{\text{CMB}} e^{-\tau} + T_S (1 - e^{-\tau})$, the observed mean differential antenna temperature relative to the CMB is [4]

$$\begin{aligned} T_b &= (1+z)^{-1} (T_S - T_{\text{CMB}}) (1 - e^{-\tau}) \\ &\simeq 26.8 \text{ mK} \left(\frac{\Omega_b h}{0.0327} \right) \left(\frac{\Omega_m}{0.307} \right)^{-1/2} \left(\frac{1+z}{10} \right)^{1/2} \left(\frac{T_S - T_{\text{CMB}}}{T_S} \right), \end{aligned} \quad (12.4)$$

where $\tau \ll 1$ is assumed (the relative correction to the linear term that we kept is $\tau/2$) and T_b has been redshifted to redshift zero. We use here the now standard notation of T_b for this final quantity. Note that the brightness temperature is simply a measure of intensity in equivalent temperature units, defined in terms of the Rayleigh–Jeans limit of the Planck spectrum:

$$I_\nu = 2k_B T_b \frac{\nu^2}{c^2}. \quad (12.5)$$

In 21-cm cosmology, the CMB is certainly deep in the Rayleigh–Jeans limit, as its Planck spectrum peaks at a wavelength of ~ 2 mm, while the observed (redshift 0) wavelengths of relevance to us here are three orders of magnitude larger.

The IGM is observable when T_S differs from T_{CMB} , which is reasonable since $T_S = T_{\text{CMB}}$ implies a kind of thermal equilibrium between the ground-state hyperfine levels of hydrogen and the CMB background, meaning that the net effect of the gas is neither absorption nor added emission above the background. The key question for 21-cm observations is thus the value of the spin temperature. For intergalactic hydrogen it is determined by three processes. First, by direct absorption and emission (both spontaneous and stimulated) of 21-cm photons from/into the

radio background (which at high redshifts is simply the CMB), the hyperfine levels of hydrogen tend to thermalize with the CMB, making the IGM unobservable. If other processes shift the hyperfine level populations away from such a thermal equilibrium, then the gas becomes observable against the CMB in emission or in absorption. In the presence of the CMB alone, the spin states would reach thermal equilibrium with $T_S = T_{\text{CMB}} = 2.725(1+z)$ K on a time-scale of $T_*/(T_{\text{CMB}}A_{10}) \simeq 3 \times 10^5(1+z)^{-1}$ yr. This time-scale is much shorter than the age of the universe at all redshifts after cosmological recombination.

On the other hand, at high densities the spin temperature comes into equilibrium with the regular, kinetic temperature T_K that describes the random velocities of the hydrogen atoms. This equilibrium is enforced by collisions, which involve energies of order $k_B T_K$, and drive T_S towards T_K [5]. Collisionally-induced transitions are effective at high redshift, but become less effective compared to the CMB at low redshift. This may seem surprising given that as the universe expands, the mean energy density of radiation decreases faster than that of matter, and the comparison here is between two-body interactions of the hydrogen atom with either a photon or a second atom. Part of the explanation is that while the total radiation energy density goes as T_{CMB}^4 (and thus decreases rapidly with time), the relevant energy density for the 21-cm coupling is that at a fixed physical wavelength of 21 cm; this is only proportional to T_{CMB} in the Rayleigh–Jeans limit of the Planck spectrum of the CMB (Eq. (12.5)). In addition, the collisional rate coefficient (see below) depends strongly on temperature in the relevant range, and it decreases very rapidly as the gas cools with time. Thus, if collisions were the only coupling mechanism of the spin temperature with the kinetic temperature, the cosmic gas would disappear at 21 cm below $z \sim 30$.

Instead, 21-cm cosmology down to $z \sim 7$ is made possible by a subtle atomic effect worked out nearly 50 years before its cosmological significance became widely recognized. This effect is 21-cm coupling as an indirect consequence of the scattering of much higher-energy Ly α photons [6, 7]. Continuum UV photons produced by early radiation sources redshift by the Hubble expansion into the local Ly α line at a lower redshift, or are injected at Ly α after redshifting and cascading down from higher Lyman lines. These photons mix the spin states via the Wouthuysen-Field (hereafter WF) effect whereby an atom initially in the $n = 1$ state absorbs a Ly α photon (of wavelength $\lambda_\alpha = 1216$ Å), and the spontaneous decay that returns it from $n = 2$ to $n = 1$ can result in a final spin state that is different from the initial one (These various energy levels are illustrated in Fig. 10.1). The WF effect drives T_S to the so-called “color temperature” T_C , defined so that the spin-flip transition rates due to Ly α photons upwards (P_{01}^α) and downwards (P_{10}^α) are related by [7]:

$$\frac{P_{01}^\alpha}{P_{10}^\alpha} = 3 \left(1 - \frac{T_\star}{T_C} \right). \quad (12.6)$$

The color temperature enters since the $0 \rightarrow 1$ and $1 \rightarrow 0$ scattering events are caused by photons with slightly different frequencies. It is the equivalent temperature of

a blackbody spectrum that would yield this transition rate ratio. In general (i.e. including the case of a non-blackbody radiation background), the color temperature is determined by the shape of the radiation spectrum near $\text{Ly}\alpha$, and is related to the photon intensity J through [8]

$$\frac{h}{k_B T_C} = \frac{2}{\nu} - \frac{d \ln J}{d \nu}. \quad (12.7)$$

Given CMB scattering (which pulls $T_S \rightarrow T_{\text{CMB}}$), atomic collisions ($T_S \rightarrow T_K$), and $\text{Ly}\alpha$ scattering ($T_S \rightarrow T_C$), the spin temperature becomes a weighted mean [7]:

$$T_S^{-1} = \frac{T_{\text{CMB}}^{-1} + x_c T_K^{-1} + x_\alpha T_C^{-1}}{1 + x_{\text{tot}}}, \quad (12.8)$$

where $x_{\text{tot}} = x_c + x_\alpha$ and the combination that appears in T_b (Eq. (12.4)) is then:

$$\frac{T_S - T_{\text{CMB}}}{T_S} = \frac{x_{\text{tot}} - T_{\text{CMB}} (x_c T_K^{-1} + x_\alpha T_C^{-1})}{1 + x_{\text{tot}}}. \quad (12.9)$$

Here we have used the notation from Barkana & Loeb (2005) [10] in terms of the coupling coefficients x_c and x_α for collisions and $\text{Ly}\alpha$ scattering, respectively. They are given by [4]¹

$$x_c = \frac{\kappa_{1-0}(T_k) n_H T_\star}{A_{10} T_{\text{CMB}}}, \quad (12.10)$$

where the collisional rate coefficient $\kappa_{1-0}(T_k)$ is tabulated as a function of T_k [12, 13], and

$$x_\alpha = \frac{4 P_\alpha T_\star}{27 A_{10} T_{\text{CMB}}}, \quad (12.11)$$

in terms of the $\text{Ly}\alpha$ scattering rate P_α . Expressed in terms of the proper $\text{Ly}\alpha$ photon intensity J_α (defined as the spherical average of the number of photons hitting a gas element per unit area per unit time per unit frequency per steradian),

$$x_\alpha = \frac{16 \pi^2 T_\star e^2 f_\alpha}{27 A_{10} m_e c T_{\text{CMB}}} J_\alpha, \quad (12.12)$$

except for a low-temperature correction (see the next section), where $f_\alpha = 0.4162$ is the oscillator strength of the $\text{Ly}\alpha$ transition.

The neutral IGM is highly opaque to resonant scattering, which involves energy transfers between the atomic motion and the photons, and tends to drive a kind of thermal equilibrium between the photon energy distribution near $\text{Ly}\alpha$ and the kinetic motion of the atoms. This makes T_C very close to T_K [14], except for another

¹Note that there was an erroneous factor of 4/3 in Eq. (12.10) in some previous publications [9–11].

low-temperature correction (see the next subsection). In the high-temperature approximation, Eq. (12.8) and Eq. (12.9) simplify to:

$$T_S^{-1} = \frac{T_{\text{CMB}}^{-1} + x_{\text{tot}} T_K^{-1}}{1 + x_{\text{tot}}}, \quad (12.13)$$

and

$$\frac{T_S - T_{\text{CMB}}}{T_S} = \frac{x_{\text{tot}}}{1 + x_{\text{tot}}} \left(1 - \frac{T_{\text{CMB}}}{T_K} \right). \quad (12.14)$$

Below $z \sim 200$, the gas is mostly thermally decoupled from the CMB and $T_K < T_{\text{CMB}}$ (until significant X-ray heating), so that 21-cm observations are possible since collisions or Ly α scattering provide an effective mechanism coupling T_S to T_K . While Eq. (12.4) gives the 21-cm brightness temperature in a fully-neutral, homogeneous universe, in the real Universe T_b fluctuates. It is proportional in general to the gas density, and in partially ionized regions T_b is proportional to the neutral hydrogen fraction. Fluctuations in the velocity gradient term in Eq. (12.2) leads to a line-of-sight anisotropy in the 21-cm signal (Sec. 12.3). Also, if $T_S > T_{\text{CMB}}$ then the IGM is observed in emission, and when $T_S \gg T_{\text{CMB}}$ the emission level saturates at a level that is independent of T_S . On the other hand, if $T_S < T_{\text{CMB}}$ then the IGM is observed in absorption, and if $T_S \ll T_{\text{CMB}}$ the absorption strength is a factor $\sim T_{\text{CMB}}/T_S$ larger (in absolute value) than the saturated emission level. In addition, once the Universe fills up with Ly α radiation and the WF effect turns on (this is the Ly α coupling transition, with its peak usually defined as the point when $x_{\text{tot}} = 1$ due mostly to x_α), the rapid rise expected during the early stages of cosmic star formation implies that soon afterwards $x_\alpha \gg 1$ and T_b saturates to a value that no longer depends on x_α . As a result of these various considerations, a number of cosmic events (Chap. 14) are expected to leave observable signatures in the redshifted 21-cm line (Chap. 15).

12.2. Low-temperature corrections

There are two corrections to the 21-cm coupling due to Ly α scattering, which can be important in low-temperature gas. Both arise from a careful consideration of the multiple scatterings of the photons near the Ly α resonance with the hydrogen atoms, and how these scatterings affect the energy distribution of the photons near the resonance, resulting in a change in the 21-cm coupling. One correction is due to a difference between the color temperature and the kinetic temperature of the gas, and the other due to a modified Ly α scattering rate. We attempt here to clear up confusion in some of the literature on this subject.

An accurate determination of the Ly α color temperature requires a careful consideration of radiative scattering including atomic recoil and energy transfer due to spin exchange. In the limit of a high optical depth to Ly α scattering (an

excellent approximation in the cosmological context),

$$T_C = T_K \left(\frac{1 + T_{\text{se}}/T_K}{1 + T_{\text{se}}/T_S} \right), \quad (12.15)$$

which differs significantly from T_K once temperatures approach T_{se} , which is given by

$$T_{\text{se}} = \frac{m_H c^2}{9k_B} \left(\frac{\lambda_\alpha}{\lambda_{21}} \right)^2 = 0.402 \text{ K}, \quad (12.16)$$

where m_H is the mass of a hydrogen atom. Equation (12.15) is easily solved simultaneously with Eq. (12.8), yielding results that have precisely the same form as Eq. (12.13) and Eq. (12.14) if we replace x_{tot} by an $x_{\text{tot,eff}}$ in which we adopt an effective value $x_{\alpha,\text{eff}} = x_\alpha/(1 + T_{\text{se}}/T_K)$.

The second effect modifies the relation between J_α (defined as the naive Ly α photon intensity, i.e. not including the modification due to multiple scattering) and the actual Ly α scattering rate P_α . The final result is to multiply Eq. (12.12) by an extra factor S_α , which depends on T_K as well as the Gunn–Peterson [15] optical depth to Ly α absorption, which for neutral gas at the cosmic mean density is

$$\tau_{\text{GP}} = \frac{\pi e^2 f_\alpha \lambda_\alpha n_{\text{HI}}}{m_e c H} = 6.62 \times 10^5 \left(\frac{\Omega_b h}{0.0327} \right) \left(\frac{\Omega_m}{0.307} \right)^{-1/2} \left(\frac{1+z}{10} \right)^{3/2}, \quad (12.17)$$

where in the second equality we used the high-redshift form of the Hubble parameter $H(z)$.

The scattering-rate correction factor S_α is due to the fact that the H atoms recoil in each scattering, and near the center of the Ly α line, frequent scatterings with atoms make the photons lose energy faster. Thus, the number of photons per unit energy at any instant is smaller than would have been expected without recoil, leading to a suppression in the scattering rate (i.e. $S_\alpha < 1$). The actual value of S_α is derived from solving the radiative transfer equation for the photons including scattering and energy losses. The result is

$$S_\alpha = e^{-0.0128(\tau_{\text{GP}}/T_K^2)^{1/3}}, \quad (12.18)$$

with T_K in Kelvin (in this equation only). Thus, the final results including both low-temperature corrections are

$$T_S^{-1} = \frac{T_{\text{CMB}}^{-1} + x_{\text{tot,eff}} T_K^{-1}}{1 + x_{\text{tot,eff}}}, \quad (12.19)$$

and

$$\frac{T_S - T_{\text{CMB}}}{T_S} = \frac{x_{\text{tot,eff}}}{1 + x_{\text{tot,eff}}} \left(1 - \frac{T_{\text{CMB}}}{T_K} \right), \quad (12.20)$$

where $x_{\text{tot,eff}} = x_c + x_{\alpha,\text{eff}}$, and

$$x_{\alpha,\text{eff}} = x_{\alpha} \left(1 + \frac{T_{\text{se}}}{T_K}\right)^{-1} \times \exp \left[-2.06 \left(\frac{\Omega_b h}{0.0327} \right)^{1/3} \left(\frac{\Omega_m}{0.307} \right)^{-1/6} \left(\frac{1+z}{10} \right)^{1/2} \left(\frac{T_K}{T_{\text{se}}} \right)^{-2/3} \right]. \quad (12.21)$$

Equation (12.20) shows that even with the low-temperature correction, whether we get 21-cm emission or absorption is determined solely by whether T_K is larger or smaller than T_{CMB} (which seems reasonable based on thermodynamics), while at a given T_K , the absolute value of T_b increases monotonically with $x_{\alpha,\text{eff}}$. The low-temperature corrections simply reduce the effective value of x_{α} and thus reduce the absolute value of T_b and delay the onset of $\text{Ly}\alpha$ coupling and $\text{Ly}\alpha$ saturation (the latter is when $T_S \rightarrow T_K$). Note that we wrote the scattering-rate correction in Eq. (12.21) in terms of T_{se} for ease of comparison with the color-temperature correction.

These results are based on Chuzhoy & Shapiro (2006) [16], who found simple and accurate final expressions based on an approximate analytical solution (that was also found earlier in a different context [17]). The calculation of S_{α} was first carried out by Chen & Miralda-Escudé (2004) [18] (based on a numerical solution to an approximate form of the radiative transfer equation developed earlier [19, 20]), but they made a numerical error and were off by about a factor of 2. Hirata (2006) [21] gave complicated fitting formulas to numerical solutions for both corrections, but the results given above agree with those formulas to within a relative error of a few percent or better within the relevant parameter range. Furlanetto & Pritchard (2006) [22] developed higher-order analytical solutions and also compared them to full numerical solutions. Contrary to statements in the literature [1], no iteration is necessary in order to include the low-temperature corrections; the results summarized in this section are accurate at all $T \gtrsim 1$ K, except at very high temperatures (> 1000 K) which in the real Universe are reached only after the $\text{Ly}\alpha$ coupling has saturated (and so these corrections no longer matter). Note also that the scattering correction factor S_{α} , while calculated slightly differently for the continuum (red-shifting) $\text{Ly}\alpha$ photons and the injected (from higher-level cascades) $\text{Ly}\alpha$ photons, has the same value in the two cases, to high accuracy.

The quantitative results are illustrated in Fig. 12.1. The scattering correction dominates over the correction from the color temperature. In practice, the observable effects of the low-temperature corrections could be important in the real Universe during the $\text{Ly}\alpha$ coupling era. These corrections affect 21-cm fluctuations only when the $\text{Ly}\alpha$ coupling is significant but has not yet saturated (since in the saturated limit, 21-cm observations are independent of x_{α} and its corrections). As long as the cosmic gas cools, the strengthening reduction in the effective x_{α} slows the rise of

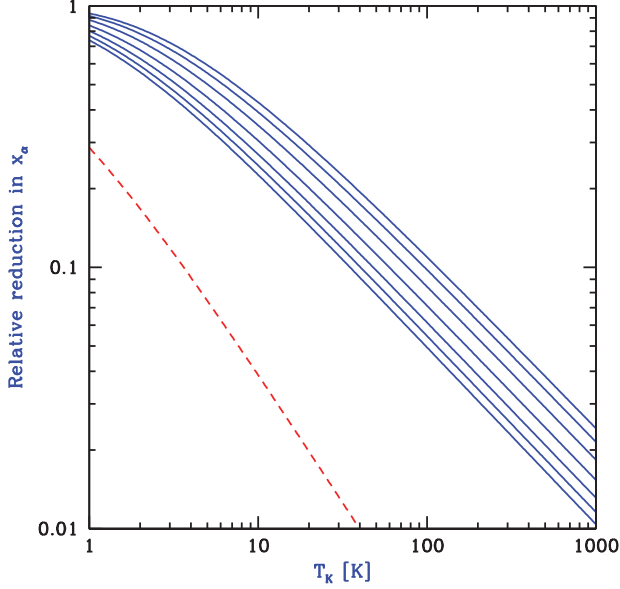


Fig. 12.1. Relative reduction in x_α , i.e. $1 - x_{\alpha,\text{eff}}/x_\alpha$, versus the kinetic gas temperature T_K . We show the total reduction (solid curves) including both the scattering and color-temperature corrections, at redshifts 7, 9, 12, 17, 25, 35, and 45 (from bottom to top), and the reduction from the modified color temperature only (dashed curve).

$\text{Ly}\alpha$ coupling; once the gas reaches its minimum temperature and begins to warm up, the declining low-temperature effect then accelerates $\text{Ly}\alpha$ saturation. In realistic models (see Chap. 14 and Chap. 15), $x_\alpha \sim 1$ is expected at $z \sim 25$, when the gas has cooled to ~ 15 K, while temperatures as low as $\sim 7 - 8$ K may be reached at $z \sim 17$ (e.g. in the plausible case of late heating), although x_α is then expected to already be fairly large. Thus, the low-temperature corrections may affect T_b by up to $\sim 20\%$ within this redshift range.

12.3. The 21-cm power spectrum and its anisotropy

As explained previously, the 21-cm signal on the sky is potentially an extremely rich dataset. This signal is intrinsically three dimensional, covering the full sky over a wide range of redshifts. If the cosmic mean 21-cm brightness temperature at some redshift is $\langle T_b \rangle$, then the 21-cm fluctuation level δT_b at wavenumber k (usually in units of mK) is defined as (compare Eq. (3.41)):

$$\delta T_b = \langle T_b \rangle \sqrt{\frac{k^3 P(k)}{2\pi^2}}, \quad (12.22)$$

in terms of the dimensionless 21-cm power spectrum $P(k)$ (i.e. the power spectrum of relative fluctuations in the 21-cm brightness temperature). Even if 21-cm

fluctuations are only measured statistically in terms of the isotropically-averaged power spectrum of fluctuations, this power spectrum versus redshift should yield a powerful dataset that can probe a wide range of the physics and astrophysics of the first stars and galaxies (as explored in detail in Chap. 15).

The fluctuations in 21-cm cosmology are potentially even richer, as a result of a particular form of anisotropy that is expected due to gas motions along the line of sight [9, 23, 24]. This anisotropy, expected in any measurement of density that is based on a spectral resonance or on redshift measurements, results from velocity compression. The point is that spectral absorption is determined directly by the velocity (along the line of sight) of gas rather than its position. As an extreme example, a slab of neutral hydrogen with no internal motions will all appear to be at the same redshift from an observer, producing enormous absorption at one particular frequency and thus appearing like a huge density enhancement at the corresponding redshift, even though the real, physical density need not be high (if the slab extends over a long distance along the line of sight).

More generally, consider a photon traveling along the line of sight that resonates with absorbing atoms at a particular point. In a uniform, expanding universe, the absorption optical depth encountered by this photon probes a particular narrow strip of atoms, since the expansion of the universe makes all other atoms move with a relative velocity that takes them outside the narrow frequency width of the resonance line. If there is a density peak, however, near the resonating position, the increased gravity will reduce the expansion velocities around this point and bring more gas into the resonating velocity width. Thus, near a density peak, the velocity gradient tends to increase the 21-cm optical depth above and beyond the direct increase due to the gas density itself. This effect is sensitive only to the line-of-sight component of the gradient of the line-of-sight component of the velocity of the gas, and thus causes an observed anisotropy in the 21-cm power spectrum even when all physical causes of the fluctuations are statistically isotropic. Barkana & Loeb (2005) [9] showed that this anisotropy is particularly important in the case of 21-cm fluctuations. When all fluctuations are linear, the 21-cm power spectrum takes the form [9]

$$P_{21\text{-cm}}(\mathbf{k}) = P_{\text{iso}}(k) + 2\mu^2 P_{\rho\text{-iso}}(k) + \mu^4 P_{\rho}(k), \quad (12.23)$$

where $\mu = \cos \theta$ in terms of the angle θ between the wavevector $\mathbf{k}$ of a given Fourier mode and the line of sight, $P_{\text{iso}}(k)$ is the isotropic power spectrum that would result from all sources of 21-cm fluctuations without velocity compression, $P_{\rho}(k)$ is the power spectrum of gas density fluctuations, and $P_{\rho\text{-iso}}(k)$ is the Fourier transform of the cross-correlation between the density and all (isotropic) sources of 21-cm fluctuations. Here the velocity gradient has led to the appearance of the density power spectrum due to their simple relationship via the continuity equation. The three power spectra can more generally be denoted according to the power of μ that multiplies each term:

$$P_{21\text{-cm}}(\mathbf{k}, z) = P_{\mu^0}(k, z) + 3\mu^2 P_{\mu^2}(k, z) + 5\mu^4 P_{\mu^4}(k, z), \quad (12.24)$$

where we have defined the coefficients according to their angle-averaged size (e.g. P_{μ^4} is defined accounting for $\langle \mu^4 \rangle = 1/5$), and have written the redshift dependence explicitly.

Given this anisotropic form, measuring the power spectrum as a function of μ should yield three separate power spectra at each redshift [9]. These probe, in turn, the 21-cm fluctuations without the velocity gradient term (through the μ -independent term); basic cosmology (through the intrinsic density power spectrum, measurable from the μ^4 term even when complex astrophysical processes contribute to the other terms); and additional information about the nature and properties of the various sources of 21-cm fluctuations (through the μ^2 term, which measures the cross-correlation between density fluctuations and the total isotropic 21-cm fluctuations).

In practice, 21-cm fluctuations on small scales are quite non-linear, and this non-linearity cannot be completely decoupled from large scales. In other words, even if the fluctuations are linear on a particular large scale, the way the fluctuations on that scale are measured is via a Fourier decomposition of the overall 21-cm fluctuations, which include non-linear, small-scale fluctuations. This small-scale averaging may to some degree cancel out, or largely result in an overall, simple bias factor, but the fact that the averaging involves non-linearity makes the interpretation of even large-scale measurements somewhat model-dependent. This is the double-edged sword of small-scale 21-cm fluctuations: on the one hand, they make 21-cm cosmology potentially a much larger dataset than CMB anisotropies [25], but on the other hand, they make 21-cm fluctuations more susceptible to non-linear effects (see the related discussion in Sec. 11.3 of non-linear limits on the accuracy of analytical models).

Numerical investigations during cosmic reionization [26–29] suggest that indeed, the decomposition of the line-of-sight anisotropy is more complex than the simple linear limit. It remains an incontrovertible fact, though, that the line-of-sight anisotropy makes 21-cm cosmology richer. The anisotropy allows three separate power spectra to be measured at each redshift, or more generally, a two-dimensional function of k and μ . At worst, the interpretation of this large dataset will be somewhat complicated and will need to be studied numerically, but in any case the anisotropy makes the 21-cm technique more powerful. There, are, moreover, two important caveats to these numerical studies. First, they focused on reionization (dominated by UV photons), which is a particularly difficult case as it makes the 21-cm fluctuations intrinsically non-linear on small scales, since the ionization fraction basically jumps from zero to unity in going from a neutral region to an H II bubble. And second, they focused on the μ^4 term and its promised yield of the primordial power spectrum; this term, though, is usually the smallest of the three anisotropic terms (as it does not benefit from the large bias of galaxies which enhances terms dominated by astrophysical radiation), so it is most susceptible to non-linear contamination.

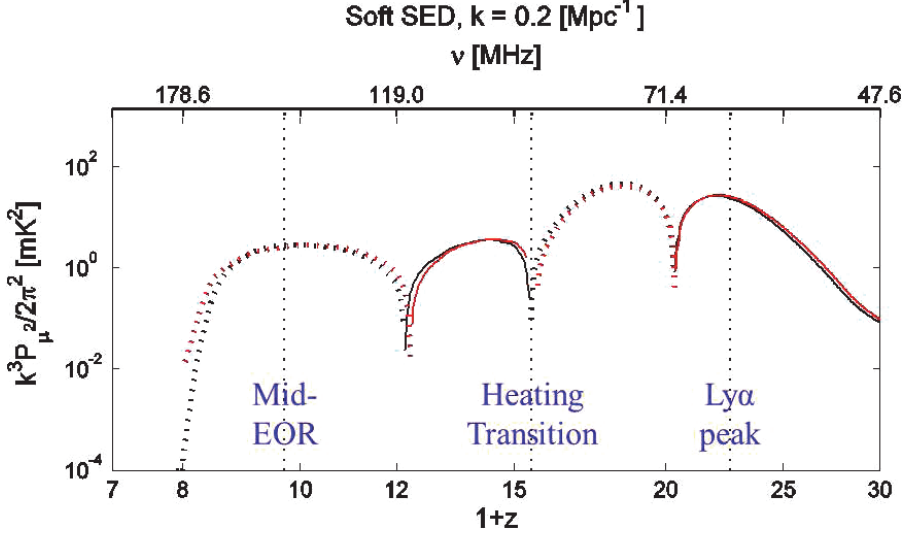


Fig. 12.2. The main anisotropic term of the 21-cm power spectrum, $P_{\mu^2}(k, z)$, shown in terms of the corresponding variance of the 21-cm fluctuations, at wavenumber $k = 0.2 \text{ Mpc}^{-1}$. The comparison of the actual value [reconstructed by fitting the form of Eq. (12.24) to mock observations] (red) with that from assuming perfect linear separation [as in Eq. (12.23)] (black) shows that this quantity withstands non-linearities and can be reconstructed accurately. This quantity, which measures the cross-correlation between density fluctuations and 21-cm fluctuations, is sometimes positive (solid lines) and sometimes negative (dashed lines), as it tracks early history like a cosmic clock. It is negative during the EOR as a direct reflection of inside-out reionization (Sec. 14.1): higher density implies more galaxies which implies less neutral hydrogen, hence an inverse cross-correlation of density and the 21-cm signal. It is positive during the Ly α coupling era, as more galaxies imply stronger Ly α radiation and a stronger 21-cm (absorption) signal. During the cosmic heating era, it changes sign at the heating transition (when the cosmic H I gas is first heated above the CMB temperature), the point at which heating a gas element switches from reducing the size of the 21-cm (absorption) signal to enhancing the size of the (emission) signal. The particular model shown here assumes cosmic heating by a soft power-law X-ray spectrum (see Sec. 14.3). From [30].

Recently, Fialkov *et al.* (2015) [30] reconsidered the anisotropic 21-cm power spectrum using a semi-numerical simulation that covered a wide period of early cosmic history. Focusing on the dominant anisotropic term (P_{μ^2}), they showed that the anisotropy is large and thus potentially measurable at most redshifts, and it acts as a model-independent cosmic clock that tracks the evolution of 21-cm fluctuations over various eras (see Fig. 12.2). Also, they predicted a redshift window during cosmic heating (at $z \sim 15$) when the anisotropy is small, during which the shape of the 21-cm power spectrum on large scales is determined directly by the average radial distribution of the flux received from X-ray sources at a typical point. This makes possible a direct and, again, model-independent, reconstruction of the X-ray spectrum of the earliest sources of cosmic heating.

The velocity gradient anisotropy that we have just discussed is well known in the context of galaxy redshift surveys [23], where it is often referred to as “redshift-space distortions”. In that case, it is used not as an additional probe of galaxies but of fundamental cosmology, since it allows a measurement of the amplitude of the velocity field (a recent example is [31]), which is related to the rate of change of the growth factor (see the end of Sec. 4.5.1.2). A similar velocity gradient anisotropy also arises in the context of the Ly α forest. In that case, measurements are mostly one-dimensional (i.e. along the line of sight), so redshift distortions are more difficult to extract, though they do affect observations [32].

An additional source of 21-cm anisotropy is the light-cone anisotropy [33]. While redshift can be converted to position in order to create three-dimensional cubes for calculating the 21-cm power spectrum, the line-of-sight direction is intrinsically different from directions on the sky. The reason is that the look-back time changes with the radial distance, and the character of the 21-cm fluctuation sources evolves with time, which results in a line-of-sight effect that introduces anisotropy. A significant anisotropy can be generated on large scales near the end of reionization [33], as has been further studied in numerical simulations [34, 42–44]. It is important to clarify a possible confusing issue here (see, e.g. a clear explanation in [34]). The light-cone anisotropy refers to 21-cm fluctuations, which will be observed by radio interferometer experiments. Interferometers measure the relative fluctuations at each redshift, and are not sensitive to the mean of the 21-cm intensity at each redshift. Mathematically, this is equivalent (for a flat sky) to not being able to measure $\mathbf{k}$ modes that point directly along the line of sight ($\mu = 1$). Once the mean at each redshift is properly removed, the light-cone effect on the power spectrum is then mainly that the measured power spectrum is a redshift average of the real power spectrum, since any frequency slice corresponds to a range of redshifts within our past light cone. Looking towards the future, the light-cone anisotropy can in principle be reduced as data become available with improved sensitivity and larger fields of views, allowing the power spectrum to be measured from thin redshift slices that minimize the light-cone effect (though the slice should not be thinner than one wavelength, which implies some remaining averaging when measuring power on large scales).

Finally, if 21-cm data are analyzed using assumed cosmological parameters that differ from the true ones, this causes an additional Alcock–Paczyński [35] anisotropy that can be used to constrain cosmological parameters [36, 37]; in particular, the technique of Eq. (12.23) can be extended, in principle permitting (in the limit of linear fluctuations) a separate probe of this anisotropy using the μ^6 term that it induces in the 21-cm power spectrum [38].

12.4. Observational aspects

Attempts to measure the cosmological 21-cm signal must deal with the much stronger foreground emission, dominated by synchrotron radiation from electrons

in the Milky Way, with other radio sources added on. Indeed, the brightness temperature of the sky for typical high-latitude, relatively quiet portions of the sky, is [1]

$$T_{\text{sky}} \sim 180 \left(\frac{\nu}{180 \text{ MHz}} \right)^{-2.6} \text{ K}. \quad (12.25)$$

This steep increase of foreground emission with decreasing frequency is the reason that 21-cm observations become more difficult with increasing redshift; distortion of the radio signal due to refraction within the Earth's ionosphere also increases with redshift, down to the critical plasma frequency of $\nu \sim 20$ MHz below which the ionosphere becomes opaque. The sky emission in Eq. (12.25) must be compared to the expected signal of typically a few tens of mK (sky averaged), with fluctuations of order several mK. The reason that this tiny signal may be observable, even on top of a foreground that is brighter by at least a factor of 10^4 , is that the foreground is produced by synchrotron emission which inherently produces a very smooth frequency spectrum.

There are a number of approaches to observing the 21-cm signal from high redshifts. The simplest, in principle, is measuring the global 21-cm signal, i.e. the sky-averaged, cosmic mean emission as a function of frequency (i.e. redshift). This can be done with a single dish (or dipole), but requires a very accurately calibrated instrument to enable foreground subtraction. Indeed, the sensitivity of a single dish [39] is

$$\Delta T \sim \frac{T_{\text{sys}}}{\sqrt{\Delta\nu t_{\text{int}}}}. \quad (12.26)$$

Assuming that the system temperature is approximately equal to that of the foreground [Eq. (12.25)], and taking a bandwidth of $\Delta\nu = 5$ MHz centered at $z = 10$ ($\nu = 129$ MHz), a sensitivity of $\Delta T = 10$ mK only requires an integration time t_{int} of 6 minutes. Thus, the real issue with global 21-cm experiments is not raw sensitivity, but the ability to clean out the smooth foreground emission to a spectral accuracy of one part in 10^4 or 10^5 . In practice, the need to subtract out the smoothly-varying foreground implies a simultaneous removal of the smoothly-varying part of the desired 21-cm signal. Thus, the absolute level of the global signal likely cannot be measured, but its variation with frequency may be measurable, particularly when the frequency gradient of the 21-cm signal is large during the rises or declines that accompany various milestones of early cosmic evolution (see Sec. 15.5).

The other main approach is to make an interferometric map of the 21-cm signal. In this case, much more information is available at each redshift than just a single mean temperature. With a sufficiently high signal-to-noise ratio, direct tomography/imaging can reveal the full spatial distribution of the 21-cm signal. However, even if the maps themselves are noisy, statistical measures such as the 21-cm power spectrum can be computed with high accuracy, and used to extract many of the most interesting aspects of cosmic dawn such as the properties of the

galaxies that existed at various times. In the case of an interferometer, one basic consideration is the achievable angular resolution θ_D , determined by the diffraction limit corresponding to the longest array baseline $D_{\max}$ [1]:

$$\theta_D \sim \frac{\lambda}{D_{\max}} \sim 7.3 \left(\frac{1+z}{10} \right) \left(\frac{D_{\max}}{1 \text{ km}} \right)^{-1}. \quad (12.27)$$

The corresponding comoving spatial resolution r_D is

$$r_D \sim 20 \left(\frac{h}{0.68} \right)^{-1} \left(\frac{1+z}{10} \right)^{1.2} \left(\frac{D_{\max}}{1 \text{ km}} \right)^{-1} \text{ Mpc}. \quad (12.28)$$

For an array of N radio antennae (or stations), each with an effective collecting area A_{eff} , the resulting field of view $\Omega_{\text{FoV}} = \lambda^2/A_{\text{eff}}$ corresponds to an angular diameter

$$\theta_{\text{FoV}} \equiv \sqrt{\frac{4\Omega_{\text{FoV}}}{\pi}} = 5.1 \left(\frac{1+z}{10} \right) \left(\frac{A_{\text{eff}}}{700 \text{ m}^2} \right)^{-1/2}. \quad (12.29)$$

The corresponding comoving distance (transverse to the line of sight) is

$$r_{\text{FoV}} \sim 0.86 \left(\frac{h}{0.68} \right)^{-1} \left(\frac{1+z}{10} \right)^{1.2} \left(\frac{A_{\text{eff}}}{700 \text{ m}^2} \right)^{-1/2} \text{ Gpc}. \quad (12.30)$$

In the line-of-sight direction, the comoving length corresponding to a bandwidth $\Delta\nu$ is [1]

$$r_{\Delta\nu} \sim 18 \left(\frac{\Delta\nu}{1 \text{ MHz}} \right) \left(\frac{1+z}{10} \right)^{1/2} \left(\frac{\Omega_m h^2}{0.141} \right)^{-1/2} \text{ Mpc}. \quad (12.31)$$

Another commonly noted quantity is the total collecting area of the array

$$A_{\text{coll}} = N A_{\text{eff}} = 1.8 \times 10^5 \left(\frac{N}{250} \right) \left(\frac{A_{\text{eff}}}{700 \text{ m}^2} \right) \text{ m}^2, \quad (12.32)$$

where we have used illustrative values based roughly on the planned first phase of the Square Kilometer Array [40] (though note that A_{eff} is actually expected to vary with frequency).

A key quantity for interferometric arrays is the sensitivity to power spectrum measurements. We assume the simple approximation of antennae distributed over a core area A_{core} in such a way that the uv -density (i.e. the density in visibility space which is equivalent to a Fourier transform of the sky) is uniform, and a single

beam (i.e. we do not include here the technique of multi-beaming which can speed up surveys). In this case, the power-spectrum error due to thermal noise is [40, 41]

$$\Delta T_{\text{PS}}^{\text{thermal}} = \sqrt{\frac{2}{\pi}} k^{3/4} [D_c^2 \Delta D_c \Omega_{\text{FoV}}]^{1/4} \frac{T_{\text{sys}}}{\sqrt{\Delta\nu} t_{\text{int}}} \frac{1}{N} \sqrt{\frac{A_{\text{core}}}{A_{\text{eff}}}}, \quad (12.33)$$

which yields an approximate value of

$$\begin{aligned} \Delta T_{\text{PS}}^{\text{thermal}} \sim 0.13 & \left(\frac{k}{0.1 \text{ Mpc}^{-1}} \right)^{3/4} \left(\frac{1+z}{10} \right)^{3.3} \left(\frac{t_{\text{int}}}{1000 \text{ hr}} \right)^{-1/2} \left(\frac{\Delta\nu}{1 \text{ MHz}} \right)^{-1/4} \\ & \times \left(\frac{250}{N} \right) \left(\frac{A_{\text{eff}}}{700 \text{ m}^2} \right)^{-3/4} \left(\frac{A_{\text{core}}}{3.8 \times 10^5 \text{ m}^2} \right)^{1/2} \left(\frac{\Omega_m h^2}{0.141} \right)^{-1/8} \text{ mK}, \end{aligned} \quad (12.34)$$

where D_c is the comoving distance to redshift z , and ΔD_c equals $r_{\Delta\nu}$ from above. The thermal noise thus increases with k , and typically dominates the expected power spectrum errors on small scales. Attempting to improve the angular resolution by increasing D_{max} would typically imply an increase in $A_{\text{core}} \propto D_{\text{max}}^2$ as well, and thus a worsening power-spectrum sensitivity at all k .

The uncertainty in comparing data to models is usually dominated on large scales by sample variance (sometimes termed “cosmic variance”), which gives a relative error that is roughly proportional to the inverse square root of the number of modes of wavenumber k that fit into the survey volume. Assuming a cylindrical volume and a bin width of $\Delta k \sim k$ [assumptions also made in Eq. (12.33)], this yields [41]

$$\Delta T_{\text{PS}}^{\text{sample}} \approx T_{\text{PS}} \sqrt{\frac{8\pi}{k^3 r_{\text{FoV}}^2 r_{\Delta\nu}}}, \quad (12.35)$$

where T_{PS} is the root-mean-square 21-cm brightness temperature fluctuation at wavenumber k . The resulting approximate value is

$$\begin{aligned} \Delta T_{\text{PS}}^{\text{sample}} \sim 0.087 & \left(\frac{T_{\text{PS}}}{2 \text{ mK}} \right) \left(\frac{k}{0.1 \text{ Mpc}^{-1}} \right)^{-3/2} \left(\frac{1+z}{10} \right)^{-1.5} \left(\frac{\Delta\nu}{1 \text{ MHz}} \right)^{-1/2} \\ & \times \left(\frac{A_{\text{eff}}}{700 \text{ m}^2} \right)^{1/2} \left(\frac{h}{0.68} \right) \left(\frac{\Omega_m h^2}{0.141} \right)^{1/4} \text{ mK}. \end{aligned} \quad (12.36)$$

We note, though, that these noise estimates (both thermal noise and sample variance) may in a sense be overestimated, since they are calculated for a narrow bandwidth at a single redshift (e.g. 1 MHz around $1+z=20$ corresponds to $\Delta z \sim 0.3$). If a theoretical model is fit to data covering a wide range of redshifts, then the model in a sense smoothes the data over the various redshifts, yielding effectively lower noise overall. Of course, this conclusion is not model-independent as it relies on the smooth variation with redshift typically assumed in any model, a smoothness that ties together, within such a combined fit, the data measured at various redshifts.

A model-independent way to try to reduce the errors would be to simply average the data over wide redshift bins, but that would erase some information about the redshift evolution, as well as features of the power spectrum that may only appear prominently at particular redshifts. A more direct observational approach is to use the flexibility available in balancing the amount of integration time spent per field (with more time leading to lower thermal noise), on the one hand, and the total number of separate fields of view observed (with more fields reducing the sample variance), on the other hand.

We also add a word of caution that the above noise estimates for interferometric arrays are only approximate, as they make the simplifying assumption of a uniform uv density. In real arrays, the uv density is usually higher on short baselines than on longer baselines, making it necessary to integrate numerically in order to calculate the expected noise accurately.

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Chapter 13

The Supersonic Streaming Velocity

Current observational efforts in 21-cm cosmology (and high-redshift astronomy more generally) are focused on the reionization era (redshift $z \sim 10$), with earlier times considered more difficult to observe. However, recent work suggests that at least in the case of 21-cm cosmology, the pre-reionization, $z \sim 20$ era of even earlier galaxies may produce very interesting signals that make observational exploration quite promising. One argument for this is based on a recently noticed effect on early galaxy formation that had been previously neglected. We discuss here this supersonic streaming velocity, which has also been reviewed elsewhere [1].

13.1. Cosmological origins

Up until recently, studies of early structure formation were based on initial conditions from linear perturbation theory. However, Tseliakhovich & Hirata (2010) [2] pointed out an important effect that had been missing in this treatment. At early times, the electrons in the ionized gas scattered strongly with the then-energetic CMB photons, so that the baryons moved together with the photons in a strongly-coupled fluid. On the other hand, the motion of the dark matter was determined by gravity, as it did not otherwise interact with the photons. Thus, the initial inhomogeneities in the universe led to the gas and dark matter having different velocities. When the gas recombined at $z \sim 1100$, it was moving relative to the dark matter, with a relative velocity that varied spatially. The root-mean-square value at recombination was ~ 30 km/s, which was supersonic (Mach number ~ 5). The streaming velocity then gradually decayed as $\propto 1/a$, like any peculiar velocity (Sec. 2.4), but remained supersonic (getting down to around Mach 2) until the onset of cosmic heating. This is true for the root-mean-square value, but the streaming velocity was lower in some regions, and up to a few times higher in others.

Figure 13.1 shows the contribution of fluctuations on various scales to the variance of the velocity difference. This highlights two important properties of this relative motion. First, there is no contribution from small scales, so that the relative

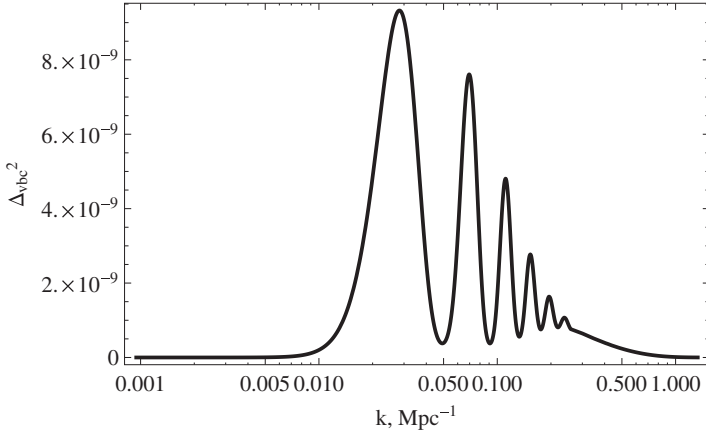


Fig. 13.1. The contribution of various scales to the mean squared velocity difference between the baryons and dark matter (at the same position) at recombination. The contribution per $\log k$ of fluctuations at wavenumber k is shown vs. k . From [2].

velocity is uniform in patches up to a few Mpc in size; the velocity is generated by larger-scale modes, up to ~ 200 Mpc in wavelength. The uniformity on small scales is critical as it allows a separation of scales between the spatial variation of the velocity (on large scales) and galaxy formation (on small scales). Each individual high-redshift mini-galaxy forms out of a small region (~ 20 kpc for a $10^6 M_\odot$ halo) that can be accurately approximated as having a uniform, local baryonic wind, or a uniform stream of baryons; the relative velocity is thus also referred to as the “streaming velocity”. The second important feature of Fig. 13.1 is the strong baryon acoustic oscillation (BAO) signature. Arising from the acoustic oscillations of the photon-baryon fluid before recombination, this strong BAO signature is a potentially observable fingerprint of the effect of this relative motion, as is further detailed below.

The relative motion between the dark matter and baryons was not in itself a surprise (it had been known for decades), but before 2010 it had not been noticed that this effect was both important and dropped within the standard approach. The standard initial conditions for both analytical calculations and numerical simulations had been generated based on linear perturbation theory, in which each $\mathbf{k}$ mode evolves independently. Indeed, the relative velocity is negligible if any single scale is considered. However, it *is* important as an effect of large scales (which contribute to the velocity difference) on small scales (which dominate early galaxy formation). Specifically, the relative motion makes it harder for small-scale overdensities in the dark matter to gravitationally accrete the streaming gas. Now, observing such small scales directly would require far higher resolution than is currently feasible in radio astronomy at high redshift. Nonetheless, the relative motion is immensely important because of its effect on star formation. Since stellar radiation strongly affects 21-cm

emission from the surrounding IGM, 21-cm cosmology offers an indirect probe of the relative velocity effect.

13.2. Effect on star formation in early halos

The effect of the streaming velocity on early star formation can be usefully separated into three effects, both for physical understanding and for the purposes of analytical modeling. This also tracks the development of the subject. The first effect of the streaming velocity on halos to be analyzed was the suppression of the abundance of halos [2]. Since the baryons do not follow the dark matter perturbations as closely as they would without the velocity effect, linear fluctuations in the total density are suppressed on small scales (where the gravitationally-induced velocities are comparable to or smaller than the relative velocity). According to the standard theoretical models for understanding the abundance of halos as a function of mass [3, 4] (Sec. 5.4), this should result in a reduction of the number density of high-redshift halos of mass up to $\sim 10^6 M_\odot$ [2], a mass range that is expected to include most of the star-forming halos at early times.

The next effect to be noted [5] was that separately from the effect on the number of halos that form, the relative velocity also suppresses the gas content of each halo that does form. It was initially claimed [5] that this second effect results in 2 mK, large-scale 21-cm fluctuations during Ly α coupling, with a power spectrum showing a strong BAO signature due to the streaming velocity effect. These conclusions were qualitatively on the mark but were later seriously revised quantitatively. In particular, it turned out [6, 7] that the gas-content effect is a minor one on star-forming halos, and is mainly important for the lower-mass gas minihalos that do not form stars.

Meanwhile, many groups began to run small-scale numerical simulations that followed individual collapsing halos subject to the streaming velocity [8–14]. In particular, two simulations [9, 10] first indicated the presence of a third effect, i.e. that the relative velocity substantially increases the minimum halo mass for which stars can form from gas that cools via molecular hydrogen cooling. The intuitive explanation is that even if a halo does manage to form (albeit with a reduced gas content), it does not contain the same dense gas core that it would in the absence of the streaming velocity. The reason is that the densest part of the halo (which is where stars first manage to form) comes together well before the rest of the halo, and is thus strongly disrupted by the streaming velocity (which is high at early times); thus, after a halo forms in the presence of the streaming velocity, it is necessary to wait longer for a dense core to develop and bring about star formation. Given these simulation results on the increase in the minimum halo mass for star formation, a physically-motivated fit [7] allowed the development of a general analytical model of early star formation that includes the effect of density as well as all three effects of the streaming velocity on star formation.

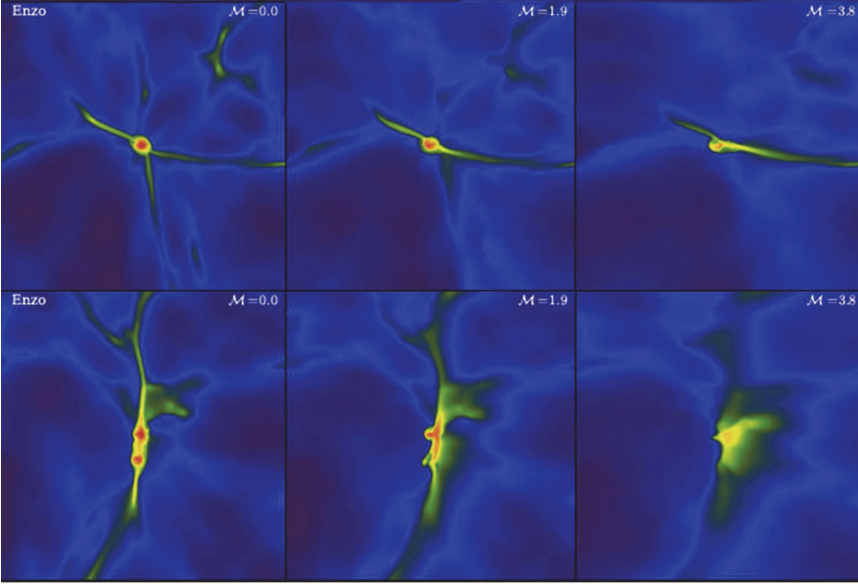


Fig. 13.2. The effect of relative velocity on individual halos, from numerical simulations (including gravity and hydrodynamics). The colors indicate the gas density, which ranges from 10^{-26}g/cm^3 (blue) to 10^{-23}g/cm^3 (red). Two halos are shown at $z = 20$, with a total halo mass of $2 \times 10^6 M_\odot$ (top panels) or $8 \times 10^5 M_\odot$ (bottom panels). Panels show the result for gas initially moving to the right with a relative velocity of 0 (left panels), 1 (middle panels), or 2 (right panels) in units of the root-mean-square value of the relative velocity. $\mathcal{M}$ indicates the corresponding Mach number at $z = 20$. From [11].

Figure 13.2 illustrates some of the results of the numerical simulation studies of the effect of the streaming velocity on galaxy formation. As expected, a larger velocity suppresses gas accretion more strongly, in particular reducing the amount of dense gas at the centers of halos. But beyond just this general trend, the relative velocity effect gives rise to very interesting dynamics on small scales. It disrupts gas accretion in an asymmetric way, so that filaments of accreting gas are disrupted more easily if they are perpendicular to the local wind direction. In addition, halos that form in regions of relatively high velocity develop supersonic wakes as they move through the wind.

13.3. Consequences

The immediate major consequence of the streaming velocity effect is the change in the large-scale distribution of the first stars in the Universe, and the resulting pattern embedded in the 21-cm sky at very high redshift. All of this is discussed below, particularly in Sec. 15.3, where the distribution of the streaming velocity field is also shown (Fig. 15.11). Here we note some other interesting consequences of the streaming velocity that have been suggested.

Although the relative velocity only affected low-mass halos at high redshifts, those halos were the progenitors of later, more massive galaxies. Thus, the streaming velocity may have indirectly left a mark on later galaxies through its influence on their star-formation histories and, thus, on their current luminosity (through their old stellar content and perhaps its feedback on the formation of younger stars). This signature may be observable in galaxy surveys, and could affect probes of dark energy through measurements of BAO positions in the galaxy power spectrum [15]; indeed, current data imply an upper limit of 3.3% on the fraction of the stars in luminous red galaxies that are sensitive to the relative velocity effect [16]. More directly, the early streaming velocity effect on star formation in dwarf galaxies could leave remnants in their properties as measured today, e.g. in the low-mass satellites of the Milky Way [17].

We note, though, that when considering these effects on later galaxies, it is important to keep in mind the modulation of star formation by other effects, in particular LW radiation (Sec. 14.2) that suppresses molecular hydrogen cooling, and reionization, which suppresses gas accretion through photoheating feedback (Sec. 14.1). These effects suppressed star formation in larger halos than the streaming velocity itself, which means that they affected later progenitors of current galaxies (containing a larger fraction of the final, present-day stellar content). The distribution of LW feedback may have reflected in part the initial relative velocity pattern [18], since the LW radiation itself was produced by stars in small halos, but reionization occurred later, likely due to more massive halos (Sec. 14.1) that were not affected much by the streaming velocity. Thus, photoheating likely did not carry a significant signature of the streaming velocity field.

Moving towards higher redshifts, as mentioned, the streaming velocity likely did not significantly affect the main stages of cosmic reionization. However, it suppressed the formation of earlier cosmic populations, perhaps including supermassive black holes at $z > 15$ [20]. More intriguing (and speculative) are ideas on opposite effects, whereby a large streaming velocity may have produced a unique environment that allowed some objects to form. A large relative velocity may have delayed star formation enough to allow a direct collapse to a massive black hole [19], or it may have produced a baryonic density peak that was sufficiently displaced from dark matter to allow the formation of an early globular cluster [21]. Moving on to the dark ages ($z > 30$), the supersonic streaming velocity had a number of significant effects on the 21-cm power spectrum at both large and small scales [22].

Recently, re-analyses of the streaming velocity effect point towards a possible boost of the effect on galaxy formation, due to advection and the coupling with density [23–25]. Note also that while the streaming velocity directly affected very small galaxies, another remnant of early cosmic history, the difference between the clustering of dark matter and baryons, has affected even the largest halos down to the present [26, 27].

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Chapter 14

Cosmic Milestones of Early Radiative Feedback

14.1. Reionization

The reionization of the Universe is an old subject. The observation of transmitted flux short-ward of the $\text{Ly}\alpha$ wavelength of quasars indicated in 1965 that the modern Universe is highly ionized [1]. While this led to a gradual growth of literature on the theoretical development of cosmic reionization (as summarized, e.g. in [2]), calculations in the context of modern cosmological models of hierarchical galaxy formation were first made in the 1990's. These included the first numerical simulations of cosmic reionization [3, 4], and analytical calculations [5–10] that mostly followed the overall, global progress of reionization, based on counting the ionizing photons from the rapidly rising star formation while accounting for recombinations. Exploration of the 21-cm signatures of reionization began in one of these numerical simulations [4] and in theoretical papers by Shaver *et al.* (1999) and Tozzi *et al.* (2000) [11, 12].

There soon began a more detailed discussion of the structure and character of reionization, important issues for a variety of observational probes of the era of reionization, especially 21-cm cosmology. A commonly-assumed simple model was that of instantaneous reionization, often adopted in calculations of the effect of reionization on the CMB. This was supported by simulations [4, 13] that showed a rapid “overlap” stage whereby the transition from individual H II regions around each galaxy to nearly full reionization was rapid ($\Delta z \sim 0.1$). Fast reionization would have made it easier to detect reionization through a sudden jump in the number of faint $\text{Ly}\alpha$ sources [14, 15] (given the strong $\text{Ly}\alpha$ absorption due to a neutral IGM).

These same simulations also found that the H II regions during reionization were typically quite small, below a tenth of a Mpc for most of reionization until a sudden sharp rise (to larger than the simulation box) once only 30% of the hydrogen mass (occupying 15% of the volume) remained neutral. Predictions made on this basis [16]

were bad news for 21-cm observations, which will find it difficult to reach the angular resolution required to see such small features within the cosmological 21-cm signal. Modeling of the effect of reionization on secondary CMB anisotropies through the kinetic Sunyaev–Zel’dovich effect (whereby the velocities of free electrons created by reionization changed the energies of the fraction of CMB photons that re-scattered) also assumed that the ionized bubble scale would be very small unless quasars were dominant [17–19].

Another basic issue about reionization is its structure/topology. At this time, both analytical models and numerical simulations [13, 20] suggested that reionization would be outside-in (with most ionizing photons leaking to the voids and reionizing them first, leaving the dense regions for later) rather than inside-out (which is when the high-density regions around the sources reionize before the low-density voids). All of the just-noted conclusions were based on numerical simulations with box sizes below 10 Mpc. A simulation of a 15 Mpc box found some ionized regions as large as 3 Mpc [21]. An even larger, 30 Mpc simulation [22] considered a field (average) region and a proto-cluster (i.e. an overdense region), and found substantial differences between their reionization histories (thus suggesting fluctuations on quite large scales), but still supported an outside-in reionization (since the proto-cluster reionized later than the field region). In hindsight, most of the results summarized in this and the previous two paragraphs were incorrect or confusing.

The now-accepted paradigm of reionization began to emerge when Barkana & Loeb (2004) [23] realized that the surprisingly strong clustering of high-redshift halos (see section Sec. 11.2) leads to H II bubbles driven by multiple clustered galaxies rather than individual galaxies¹ (see Fig. 14.1 and Fig. 14.2). This clustering is significant even on scales of tens of Mpc, leading to typical bubble sizes during reionization that are larger than the total box size of most numerical simulations of reionization at the time. The strong bias of high-redshift galaxies also settled the issue of the topology of reionization [23], showing that it is inside-out; while the recombination rate was higher in overdense regions because of their higher gas density, these regions still reionized first, despite the need to overcome the higher recombination rate, since the number of ionizing sources in these regions was increased even more strongly as a result of the strong bias of galaxies.² The outside-in picture, though, is still useful, as it seems likely to apply to the internal structure of individual H II bubbles and to the post-reionization universe. Another important revision was in the common view of the effect of reionization on the abundance of dwarf galaxies in various environments [23].

¹This paper [23] was first submitted in August 2003 but was only published 11 months later due to initial resistance to its novel conclusions.

²Quantitatively, the number of hydrogen atoms that must be initially ionized in each region is proportional to its density, i.e. the effective linear bias [Eq. (11.2)] for this quantity is unity. The number of recombinations that must be overcome goes as density squared, so its effective bias is 2. The high-redshift galaxies that are thought to have sourced reionization likely had a bias above 2 throughout reionization, with a more typical value of 5 or 10.

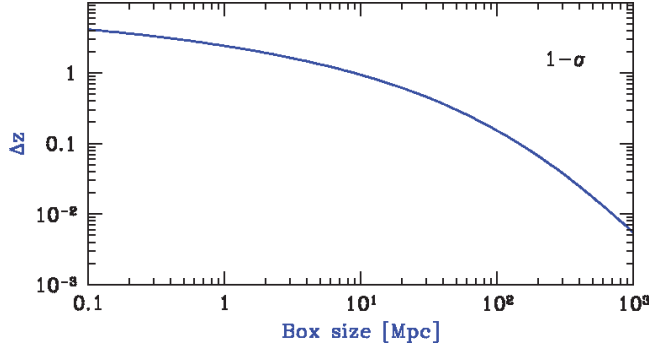


Fig. 14.1. Cosmic 1σ scatter in the redshift of reionization, or any other phenomenon that depends on the fraction of gas in galaxies, versus the size of a rectangular region (in the Universe or in a simulation). When expressed as a shift in redshift, the scatter is predicted to be approximately independent of the typical mass of galactic halos. Regions of size 10 Mpc are not representative and do not yield an overall picture of reionization, since different regions of that size reionize at redshifts that differ by a 1σ scatter of $\Delta z \sim 1$. One hundred Mpc boxes are required in order to decrease Δz to well below unity (~ 0.15). From [23].

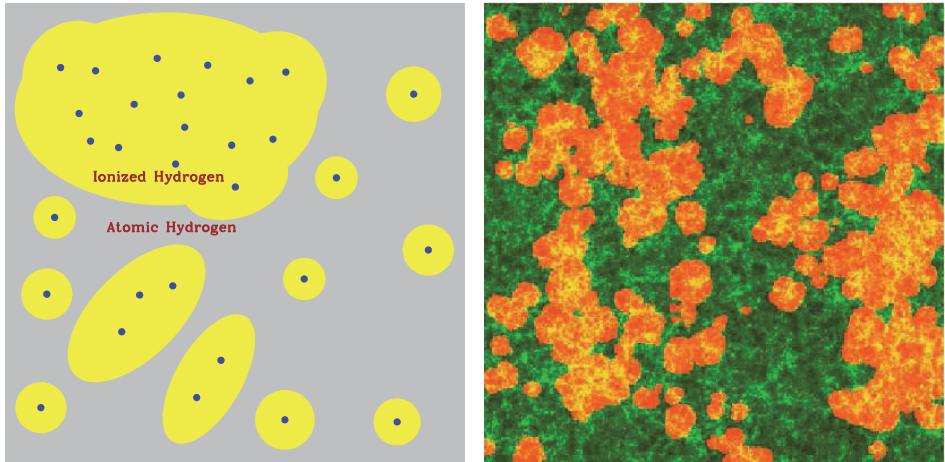


Fig. 14.2. During reionization, ionized bubbles were created by clustered groups of galaxies [23]. The illustration (left panel, from [24]) shows how regions with large-scale overdensities formed large concentrations of galaxies (dots) whose ionizing photons produced large ionized bubbles. At the same time, other large regions had a low density of galaxies and were still mostly neutral. A similar pattern has been confirmed in large-scale numerical simulations of reionization (e.g. the right panel shows a two-dimensional slice from a 150 Mpc simulation box [25]). Multiple-source bubbles likely dominated the ionized volume from as early as $z \sim 20$ [26].

The next big step was taken by Furlanetto *et al.* (2004) [27], who created an analytical model for the distribution of H II bubble sizes (Fig. 14.3), based on an ingenious application of the extended Press–Schechter model [28]. This showed how the typical size rises gradually during reionization, from a few Mpc to tens

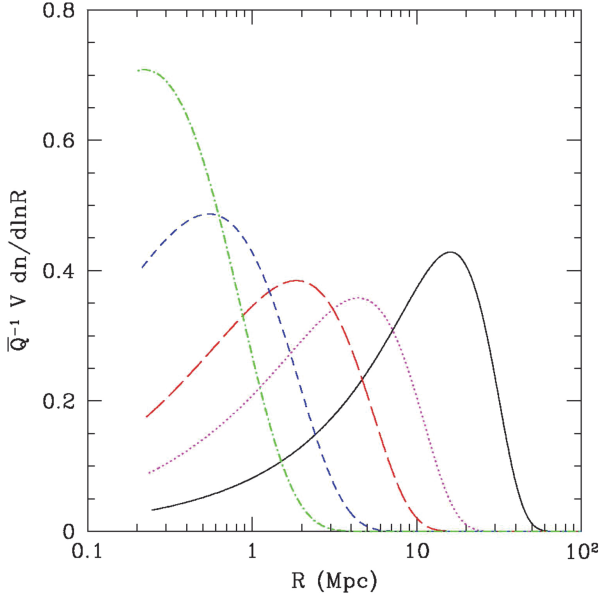


Fig. 14.3. Distribution of H II bubble sizes during reionization. The fraction of the ionized volume in bubbles of radius R is shown per $\log R$ interval. Dot-dashed, short-dashed, long-dashed, dotted, and solid lines are for $z = 18, 16, 14, 13$, and 12 , respectively, in a model in which the cosmic ionized fraction at these times is $0.037, 0.11, 0.3, 0.5$, and 0.74 , respectively. From [27].

of Mpc during the main stages, and allowed an estimate of the resulting 21-cm power spectrum during reionization. This picture of reionization based on semi-analytic models [23, 27] was then confirmed by several numerical simulations that reached sufficiently large scales with boxes of ~ 100 Mpc in size (e.g. [29–31]). The simulations indeed showed the dominance of large bubbles due to large groups of strongly-clustered galaxies, though it should be noted that the price of such large boxes was (and remains) a limited ability to resolve the small galaxies that were likely the dominant sources of reionization.

This realization, that reionization was characterized by strong fluctuations on large scales even if the individual galaxies that caused it were small, has been very important and influential. It has helped motivate the large number of observational efforts currently underway in 21-cm cosmology (Chap. 10), since large-scale fluctuations are easier to detect [as they do not require high angular resolution; see Eq. (12.34)].

Today there remain some major uncertainties about reionization that will likely only be resolved by 21-cm measurements (Sec. 15.1). In terms of the overall timing, the best current constraint comes from large-angle polarization measurements of the CMB which capture the effect of the re-scattering of CMB photons by the reionized IGM. The latest measured optical depth of $5.5 \pm 0.9\%$ [119] implies (Sec. 4.8.5) a reionization midpoint at a redshift of $7.5 - 9$ in realistic models (with reionization

completing somewhere in the range $z = 6 - 8$). However, the best-fit optical depth has changed substantially with every new measurement (declining over time), and in general it is more difficult to constrain small values of the optical depth since the corresponding reionization signature on the CMB is then smaller compared to systematic errors. The CMB results do strongly limit the high-redshift onset of reionization, with a limit of less than $\sim 10\%$ completion by $z = 10$ [33]. There have long been hints of a late end to reionization at $z \sim 6$ [34–38], but they have been controversial due to the expected large fluctuations in the cosmic ionizing background even after full reionization of the low-density IGM [39–43].

As far as the typical halo masses that hosted the dominant sources of reionization, it is expected that Lyman–Werner radiation dissociated molecular hydrogen early on [44], so that by the central stages of reionization star formation required atomic cooling, with a minimum halo mass for star-formation of $\sim 10^8 M_\odot$. As reionization proceeded, the hot gas within ionized regions raised the gas pressure and prevented it from falling into small gravitational potential wells; this photoheating feedback gradually eliminated star formation in halos up to a mass of $\sim 3 \times 10^9 M_\odot$, as has been studied in many calculations and numerical simulations [4, 45–56]. In particular, this means that an era of active star formation in dwarf galaxies prior to reionization may be observable directly with next-generation telescopes [57, 58], or in the star formation histories of massive high-redshift galaxies [59], although this depends also on the effectiveness of supernova feedback in small galaxies [60, 61].

Another interesting issue related to reionization is that of minihalos, i.e. low-mass halos that collect gas but do not form stars due to the lack of sufficient cooling. These minihalos formed in large numbers, clustered strongly around ionizing sources, and contained enough gas to effectively block most ionizing photons [62, 63]. However, the minihalos naturally photoevaporated once engulfed by H II regions [64, 65], making their effect on reionization (which they delay) and on 21-cm emission only modest [66, 67]. We note that due to their low masses, minihalos were also strongly affected by the baryon–dark matter streaming velocity (Chap. 13).

14.2. Ly α coupling and Lyman–Werner feedback

The general course of cosmic history as relevant to 21-cm cosmology was outlined in Chap. 10, and the physics of the 21-cm transition (including Ly α coupling) was described in detail in Chap. 12. Here we briefly summarize Ly α coupling and LW feedback, as they are among the most important observable events in early cosmic history.

The IGM can be observed in 21-cm emission or absorption, relative to the CMB background, only if the hyperfine levels of the hydrogen atom are not in equilibrium with the CMB. This means that the spin temperature must differ from the CMB temperature. At the highest redshifts, atomic collisions overcome the scattering of CMB photons and drive the spin temperature to the kinetic temperature of the

gas. However, this becomes ineffective at $z \sim 30$, and the spin temperature then approaches the CMB temperature. Luckily for 21-cm cosmologists, stellar Ly α photons come to the rescue [68], moving the spin temperature back towards the kinetic temperature through the indirect Wouthuysen-Field effect [69, 70]. The Ly α coupling era refers to the time during which the Ly α flux reaches and passes the level needed for effective 21-cm coupling.

Unlike reionization and heating, Ly α coupling and Lyman–Werner (LW) feedback are not cosmic events that change the overall state of the IGM. Ly α coupling is basically a 21-cm event, and it is important because of the prospect of detecting 21-cm emission from the early era ($z \sim 20 - 30$ [71, 72]) of Ly α coupling. A 21-cm observation of Ly α coupling (see Sec. 15.2 for more details) is the only currently feasible method of detecting the dominant population of galaxies from such high redshifts and measuring their properties, either through a global 21-cm detection of the strong mean absorption signal or by interferometric measurement of the substantial 21-cm fluctuations expected from this era [73]. While still far from the very first stars at $z \sim 65$ [74, 75], this is the highest redshift range currently envisioned for observing the dominant galaxy population, a feat which would be very exciting.

LW feedback is a major feedback effect on the first stars. It indirectly affects the IGM and the 21-cm sky through its effect on the radiative output from stars (including Ly α , X-ray, and ionizing radiation). LW feedback dissociates molecular hydrogen and thus it ended star formation driven by molecular cooling [44] in halos of $\sim 10^6 M_\odot$ [76, 77]. If the overall (time-averaged) star-formation efficiency in such small, early halos was significant, then their LW radiation is expected to have produced significant feedback early on ($z \sim 20 - 25$) [44, 71, 78, 79], at a time when these halos still dominated the global star formation. This feedback strengthened gradually as the LW intensity increased, as has been found in numerical simulations that imposed a LW background on forming early galaxies (either constant with time [80–82] or increasing more realistically [83]). Because of its gradual rise, LW feedback did not actually halt or reduce the global star formation, but it did slow down the otherwise rapid rise of star formation at high redshifts. Like other inhomogeneous negative feedbacks, LW feedback increased cosmic equality by first suppressing the sites of earliest star formation [71, 78, 79] (Fig. 14.4). While some LW photons reached out to a distance of ~ 100 Mpc from each source, the feedback was more local than that; emission from distant sources was absorbed more weakly, so that half the effective LW flux seen at a given point came from sources within ~ 15 Mpc away (Fig. 14.5).

A discussion of the 21-cm signatures of the Ly α coupling and LW feedback eras is deferred to Sec. 15.2. We note that in this topic it is essential to include the baryon–dark matter streaming velocity (Chap. 13) as well, since it affects the same halos as the LW feedback, and these same halos may have dominated star formation during the Ly α coupling era.

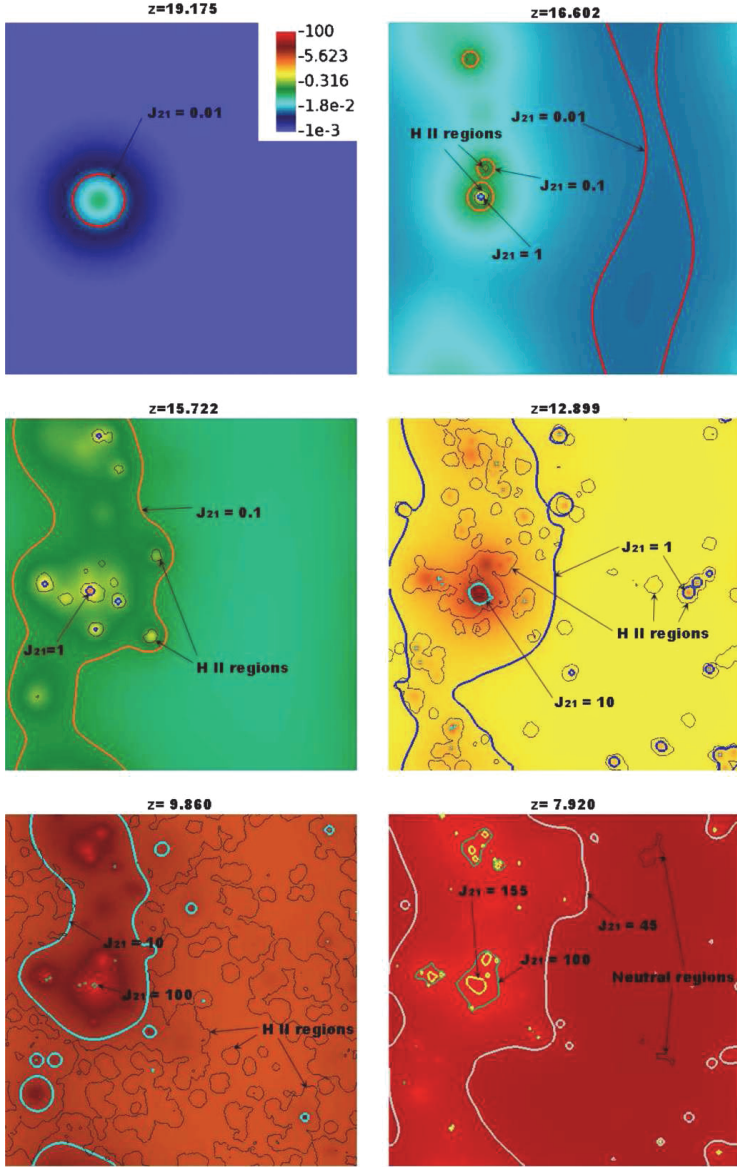


Fig. 14.4. Spatial images from a simulation showing the isocontours of patchy reionization and the patchy H_2 -dissociating background on a planar slice through a box of volume $(35/h \text{ Mpc})^3$ at various epochs. The level of $J_{\text{LW},21}$ (the LW photon intensity in units of $10^{-21} \text{ erg cm}^{-1} \text{ s}^{-1} \text{ Hz}^{-1} \text{ sr}^{-1}$) on the grid is depicted by various colors, with the range $[10^{-3} - 10^2]$ shown on the inset of the top-left panel. On top of each $J_{\text{LW},21}$ color map, contours of thick colored lines represent different $J_{\text{LW},21}$ levels (red, orange, blue, cyan, and green corresponding to $J_{\text{LW},21} = 0.01, 0.1, 1, 10, \text{ and } 100$, respectively). The black lines represent ionization fronts. From [78].

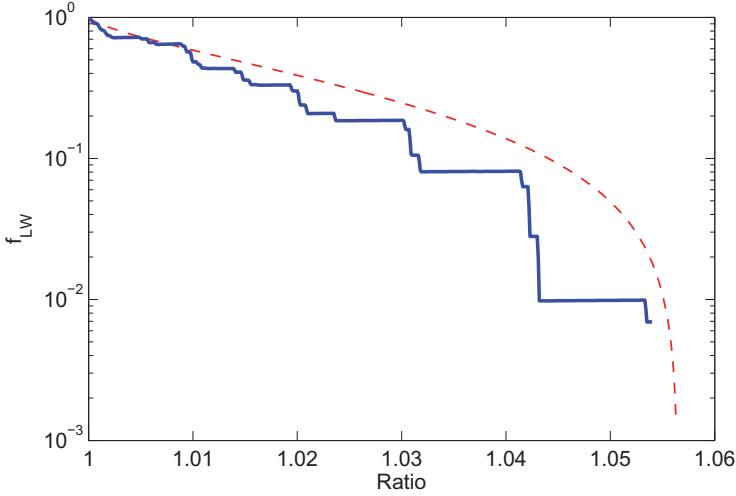


Fig. 14.5. The relative effectiveness of causing H_2 dissociation in an absorber at z_a due to stellar radiation from a source at z_s , shown versus the ratio $R \equiv (1 + z_s)/(1 + z_a)$ since in this form this function is independent of redshift. The complex result (solid curve) incorporates the expected stellar spectrum of Population III stars [73, 84], along with the full list of 76 relevant LW lines [44]. Beyond the max shown $R = 1.054$ (which corresponds to 104 comoving Mpc at $z = 20$), f_{LW} immediately drops by five orders of magnitude. Also shown is a commonly used approximation [78] (dashed curve) which is based on a flat, averaged LW spectrum. Both functions are normalized to unity at $R = 1$. From [79].

14.3. Cosmic heating

Before discussing heating in the context of 21-cm cosmology, we begin with a brief summary of the basic physics of X-ray heating. The comoving mean free path of an X-ray photon, to photoelectric absorption in a universe of neutral fraction x_{HI} , is³ [85]

$$\lambda_X \approx 51 x_{\text{HI}}^{-1} \left(\frac{1+z}{10} \right)^{-2} \left(\frac{E}{0.5 \text{ keV}} \right)^3 \text{ Mpc}. \quad (14.1)$$

For photons of energy $E \gtrsim 1 \text{ keV}$, λ_X becomes a significant fraction of the horizon (Eq. (2.45)), and in that case cosmological redshift effects lead to a substantial loss of energy between emission and absorption (plus there is a significant time delay between these two events). Once the X-rays are absorbed, the resulting (primary) fast electrons then interact with the surrounding gas through the processes of collisional excitation, ionization, and electron-electron scattering. These secondary processes quickly distribute the original X-ray energy into ionization (of hydrogen and helium in the IGM), heating (i.e. thermalized energy), and excitation (which

³In Eq. (14.1), the power-law dependence of λ_X on x_{HI} is -1 ; it has sometimes been incorrectly listed as $+1/3$ [85] or $-1/3$ [86].

results in low energy photons that then escape, so that the energy is effectively lost). The fraction of energy that goes into heating varies with the ionization fraction of the background medium, from around a third of the energy in a neutral medium up to nearly all of the energy in a highly ionized one [85, 87–89].

It has long been known that the Universe was reionized at an early time (Sec. 14.1) and thus heated to at least $\sim 10,000$ K by the ionizing photons. While reionization was a major phase transition in the IGM, the question of whether the gas had been radiatively pre-heated prior to reionization is also important. Significant pre-heating of the IGM directly affects 21-cm observations, and also produces some photoheating feedback (though much weaker than that due to reionization).

The dependence of the 21-cm brightness temperature on the kinetic temperature T_K of the gas takes the form $T_b \propto [1 - T_{\text{CMB}}/T_K]$ (Eq. (12.14) or Eq. (12.20)). Thus, the midpoint of the heating era, or the central moment of the “heating transition”, refers to the moment when the mean gas temperature is equal to that of the CMB, so that the cosmic mean T_b is zero; actually, the latter would be true in a universe with purely linear fluctuations, but non-linearities delay the time when $\langle T_b \rangle = 0$ by an extra $\Delta z \sim 0.5$ [79]. Also, clearly T_b is more sensitive to cold gas than to hot gas (relative to the CMB temperature). Indeed, at early times the 21-cm absorption can be very strong (depending on how much the gas cools), but at late times, once $T_K \gg T_{\text{CMB}}$, T_b becomes independent of T_K and the 21-cm emission is said to be in the “saturated heating” regime.

For a long time it was confidently predicted that the universe was well into the saturated heating regime once cosmic reionization got significantly underway. The stage for this widespread belief was set by the landmark paper in 21-cm cosmology by Madau *et al.* (1997) [68]. They considered several possible heating sources, mainly X-rays from quasars (later observed to disappear rapidly at $z > 3$, e.g. [90]) and heating from Ly α photons (later shown to be negligibly small [91–93]). However, stellar remnants — particularly X-ray binaries (Fig. 14.6) — have become the most plausible source of cosmic heating. This is the result of a combination of basic facts: 1) X-rays travel large distances even through a neutral IGM; 2) Large populations of X-ray binaries should have formed among the stellar remnants associated with the significant cosmic star formation that we know must have occurred in order to reionize the universe; 3) Observations of the local Universe suggest not only that X-ray binaries form wherever star formation is found, but that their relative populations increase by an order of magnitude at the low metallicity expected for high-redshift galaxies [94–98].

Even with X-ray binaries as the plausible source, the common expectation of saturated heating before reionization had remained, and had been assumed in many mock analyses made in preparation for upcoming data ([99] is a recent example). A key reason for this is that until recently, calculations of cosmic X-ray heating [86, 100–103] had assumed power-law spectra that place most of the X-ray energy at the low-energy end, where the mean free path of the soft X-rays is relatively

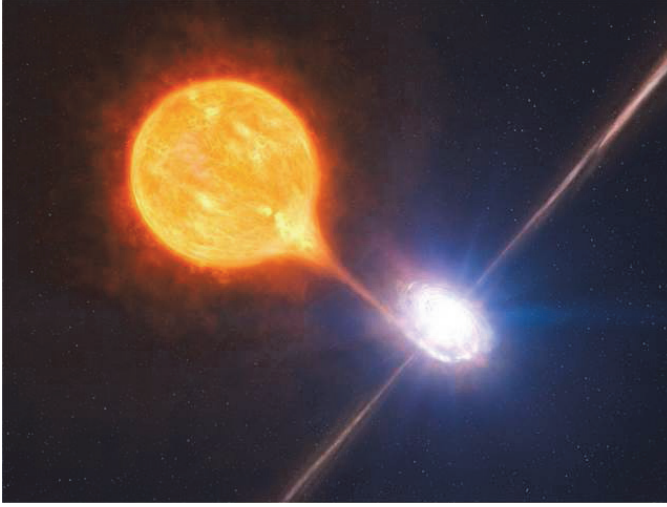


Fig. 14.6. The most plausible sources for cosmic heating before reionization are early X-ray binaries, dominated by black-hole binaries [95] like the one illustrated here, where material from a companion spills onto a black hole, resulting in X-ray emission from its accretion disk. Credit: ESO drawing from http://en.wikipedia.org/wiki/File:A_stellar_black_hole.jpg.

short. This means that most of the emitted X-rays are absorbed soon after they are emitted, before much energy is lost due to cosmological effects. The absorbed energy is then enough to heat the gas by the time of reionization to ~ 10 times the temperature of the CMB [104].

However, Fialkov *et al.* (2014) [104] recognized that the assumed X-ray spectrum is a critical parameter for both the timing of cosmic heating and the resulting 21-cm signatures. The average radiation from X-ray binaries is actually expected to have a much harder spectrum (Fig. 14.7) whose energy content (per logarithmic frequency interval) peaks at ~ 3 keV. Photons above a (roughly redshift-independent) critical energy of ~ 1 keV have such a long mean free path that by the start of reionization, most of these photons have not yet been absorbed, and the absorbed ones came from distant sources that were effectively dimmed due to cosmological redshift effects. This reduces the fraction of the X-ray energy absorbed as IGM heat by about a factor of 5, enough to push the moment of the heating transition into the expected redshift range of cosmic reionization (and thus, we will refer to this case as late heating). For this and other reasons, the spectrum of the X-ray heating sources is a key parameter for 21-cm cosmology, as further discussed in Sec. 15.3.

Based on low-redshift observations, other potential X-ray sources appear subdominant compared to X-ray binaries. One such source is thermal emission from hot gas in galaxies, which has a relatively soft X-ray spectrum. Its X-ray luminosity in local galaxies [108] is (for a given star-formation rate) about a third of that of X-ray binaries. Given the above-mentioned order-of-magnitude increase expected in the emission from X-ray binaries at high redshift, the thermal gas would have

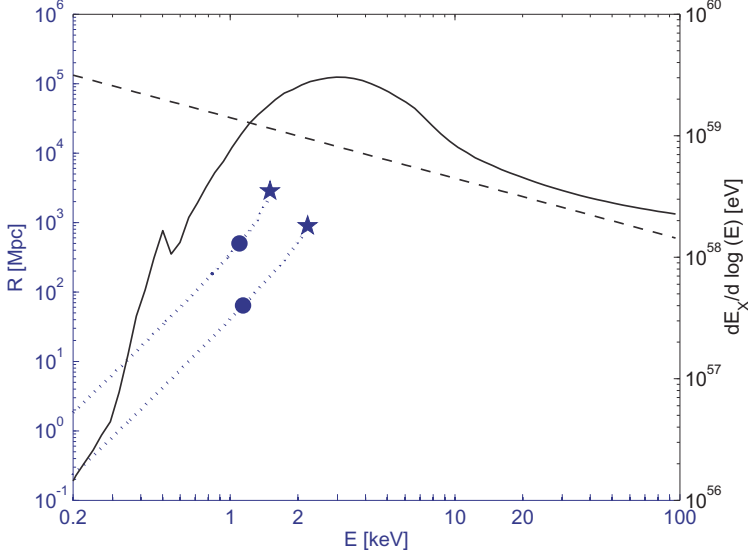


Fig. 14.7. X-ray spectra, mean free paths, and horizons. The expected spectrum of X-ray binaries at high redshift (solid curve) from population synthesis models [95, 105] is compared with the soft power-law spectrum (dashed curve) adopted until recently [86, 100–103]. Both indicate the distribution into X-ray photons with energy E of the total X-ray energy E_X produced per solar mass of newly-formed stars. The X-ray emission of X-ray binaries should be dominated by the most massive systems in their high (that is, bright) state [95], which is dominated by thermal disk emission, with little emission expected or seen [105–107] below 1 keV. Also shown are the mean free paths (dotted curves) of X-ray photons arriving at $z = 10$ (top) or $z = 30$ (bottom). For each of these redshifts, also indicated are the effective horizon for X-rays (defined as a $1/e$ drop-off, like a mean free path) from the combined effect of cosmological redshift and time retardation of sources (●), and the distance to $z = 65$ (★), the formation redshift of the first star [74, 75] (at which the mean free path curves are cut off). Note the separate y axes that indicate energy content for the spectra (right) or comoving distance for the other quantities (left). From [104].

to be highly efficient at high redshift in order to contribute significantly. Also, some theoretical arguments suggest that X-rays produced via Compton emission from relativistic electrons in galaxies could be significant at high redshift [109], though again the increase would have to be very large compared to such emission in low-redshift sources; the expected spectrum in this case (flat from ~ 100 eV to ~ 100 GeV) would deliver most of the energy above 1 keV and thus count as a hard spectrum in terms of 21-cm signatures. Another possible heating source, large-scale structure shocks, is likely ineffective [110–112].

A natural X-ray source to consider is the population of bright quasars. As noted above, while quasars are believed to dominate the X-ray background at low redshift [113], their rapid decline beyond $z \sim 3$ [90] suggests that their total X-ray luminosity (including an extrapolation of their observed luminosity function) is sub-dominant compared to X-ray binaries during and prior to reionization [95]. The rarity of quasars at early times is natural since they seem to be hosted mainly by

halos comparable in mass to our own Milky Way; the Ly α absorption signature of gas infall provides direct evidence for this [114]. More promising for early heating, perhaps, is the possibility of a population of mini-quasars, i.e. central black holes in early star-forming halos. This must be considered speculative, since the early halos were so small compared to galactic halos in the present universe that the corresponding black-hole masses are expected to fall in a very different range from observed quasars, specifically within the intermediate black-hole range ($10^2 - 10^4 M_\odot$) that local observations have probed only to a limited extent [115]. Thus, the properties of these mini-quasars are highly uncertain, and various assumptions can allow them to produce either early or late heating [93, 116]. Local observations can be used to try to estimate the possible importance of mini-quasars. An internal feedback model that is consistent with observations of local black-hole masses as well as high-redshift quasar luminosity functions [117] indicates a mini-quasar contribution that is somewhat lower than X-ray binaries [104], though the uncertainties are large. Regarding the spectrum, standard models of accretion disks [118] around black holes predict that the X-ray spectrum of mini-quasars [116] should peak at 1 – 5 keV, making it a hard spectrum for cosmic heating that is quite similar to that of X-ray binaries.

Regardless of the source of X-rays, an important parameter is the degree of absorption in high-redshift halos compared to locally observed galaxies. If we assume that the gas density in high-redshift halos increases proportionally with the cosmic mean density, then the column density through gas (within a galaxy or a halo) is proportional to $(1+z)^2 M_{\text{halo}}^{1/3}$. This simple relation suggests that absorption of X-rays should increase at high redshift, since the redshift dependence should have a stronger effect than the decrease of the typical halo mass. However, complex astrophysics could substantially affect this conclusion, since the lower binding energy of the gas in low-mass halos could make it easier to clear out more of the blockading gas. Given the large uncertainty in internal absorption (on top of the other uncertainties in source properties), it is likely that only 21-cm observations will determine the precise characteristics of the high-redshift sources of cosmic heating.

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Chapter 15

21-cm Signatures of the First Stars

Ongoing and planned interferometric observations in 21-cm cosmology hope to reach a sub-mK sensitivity level [1, 2] (see also Chap. 10). The best current observational upper limit is from PAPER [3]: 22.4 mK at a wavenumber range of $k = 0.1 - 0.35 \text{ Mpc}^{-1}$ at $z = 8.4$, around an order of magnitude away from plausible predictions (or two orders of magnitude in terms of the power spectrum). Global 21-cm experiments (measuring the total sky spectrum) are also being pursued, with the best result thus far (from the EDGES experiment) [4] being a lower limit of $\Delta z > 0.06$ for the duration of the reionization epoch. In the next few sections we focus on 21-cm fluctuations, and consider global experiments separately in Sec. 15.5.

15.1. 21-cm signatures of reionization

In Sec. 14.1 we discussed the important realizations that reionization was driven by groups of galaxies, the early galaxies were strongly clustered on large scales, and reionization had an inside-out topology. These features of reionization should all be observable with 21-cm cosmology. Figure 15.1 shows an example of 21-cm maps during reionization, as predicted by numerical simulations; a semi-numerical model gives a quite similar reionization field though it differs in the fine details. Another example is shown in Fig. 15.2, which is from a simulation that computes the ionization, $\text{Ly}\alpha$, and X-ray fields.

The typical evolution of the 21-cm power spectrum during cosmic reionization is illustrated in Fig. 15.3, using an analytical model [8] that was shown to be in reasonable agreement with numerical simulations. Early on, when the cosmic ionized fraction is $\sim 10\%$, the 21-cm power spectrum simply traces the baryon density power spectrum (assuming here the limit of saturated $\text{Ly}\alpha$ coupling and saturated heating). As reionization advances, H II bubbles form around individual sources and begin to overlap between nearby sources, giving the 21-cm power spectrum an extra hump on large scales, with the corresponding k gradually decreasing as the typical size of the bubbles increases. At the final stages of reionization, the 21-cm intensity

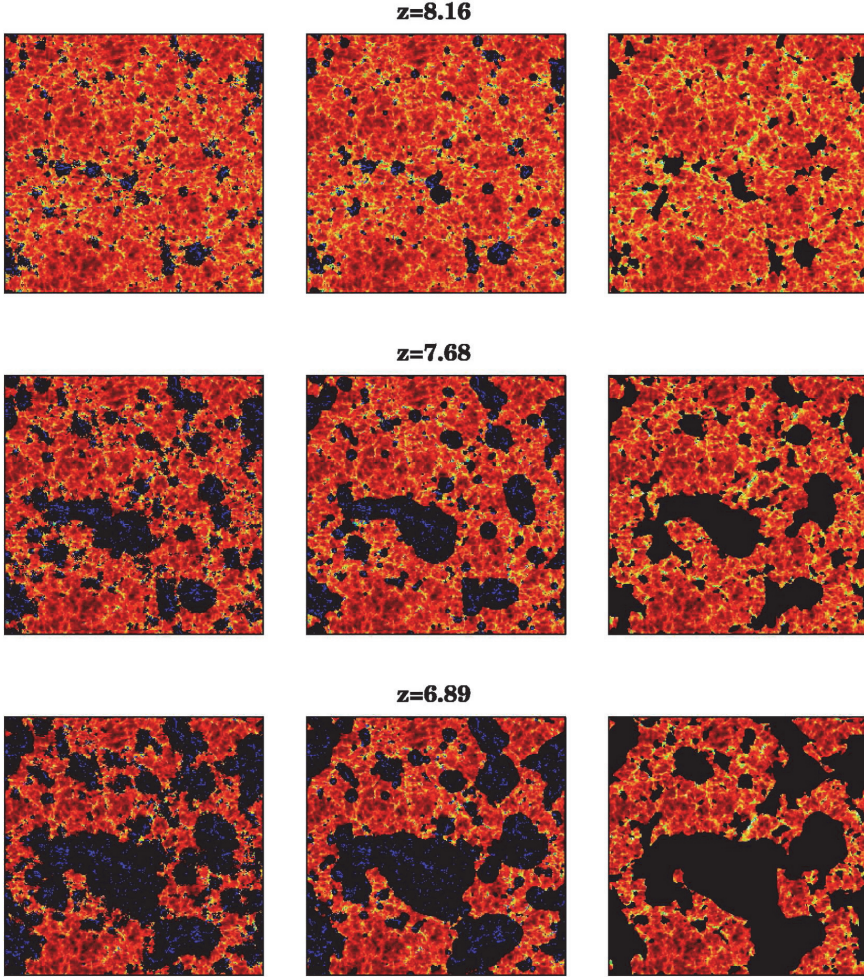


Fig. 15.1. 21-cm maps during reionization, in radiative transfer simulations versus a semi-numeric approach. Each map is 94 Mpc on a side and 0.36 Mpc deep. The ionized fractions are 0.11, 0.33, and 0.52 for $z = 8.16$, 7.26, and 6.89, respectively. Left column: Radiative transfer calculation with ionizing sources (blue dots). Middle column: Halo smoothing procedure with sources from the N-body simulation. Right column: Matching semi-numerical model based on [5] and using the initial, linear dark matter overdensity. From [6].

probes the distribution of remaining neutral gas in large-scale underdensities, and at the very end, atomic hydrogen remains only within galaxies. Figure 15.3 also illustrates how the 21-cm power spectrum can be used to probe the properties of the galaxies that are the sources of reionization. By artificially setting various values for the minimum circular velocity (or mass) of halos that dominate star formation, it is possible to simulate cases where small galaxies dominate or where large galaxies do (the latter case illustrating a situation where internal feedback is highly effective

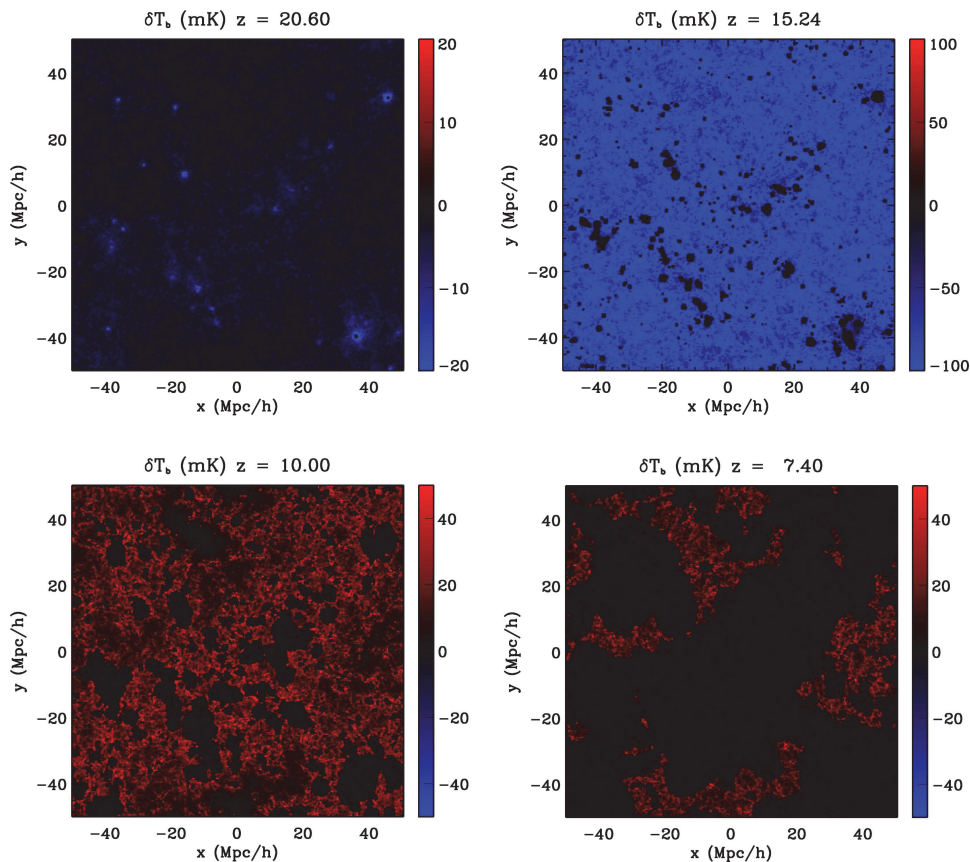


Fig. 15.2. 21-cm maps from a $100/h$ Mpc simulation box that includes inhomogeneous Ly α and X-ray radiation fields, in addition to reionization. The ionized fractions are 0.0002, 0.03, 0.35, and 0.84 for $z = 20.60$, 15.24, 10.00, and 7.40, respectively. From [7].

within small galaxies). Placing a fixed total amount of ionizing intensity within a smaller number of more massive halos has a number of effects on the 21-cm power spectrum; large halos are rarer and more strongly biased/clustered, leading to a higher power spectrum (in amplitude), a more prominent H II bubble bump that extends to somewhat larger scales, and a more rapid reionization process (in terms of the corresponding redshift range).

An important question is how to fit the 21-cm data that are expected soon from the cosmic reionization era. In general, the 21-cm power spectrum during reionization is a complex superposition of the fluctuations in density and ionization (and possibly heating; see Sec. 15.4); in order to interpret it quantitatively and reconstruct the history of reionization and of early galaxy formation, a flexible model is needed. Fitting to data cannot be done directly with numerical simulations, and is difficult even with a faster-running semi-numerical code. Thus, the first maximum

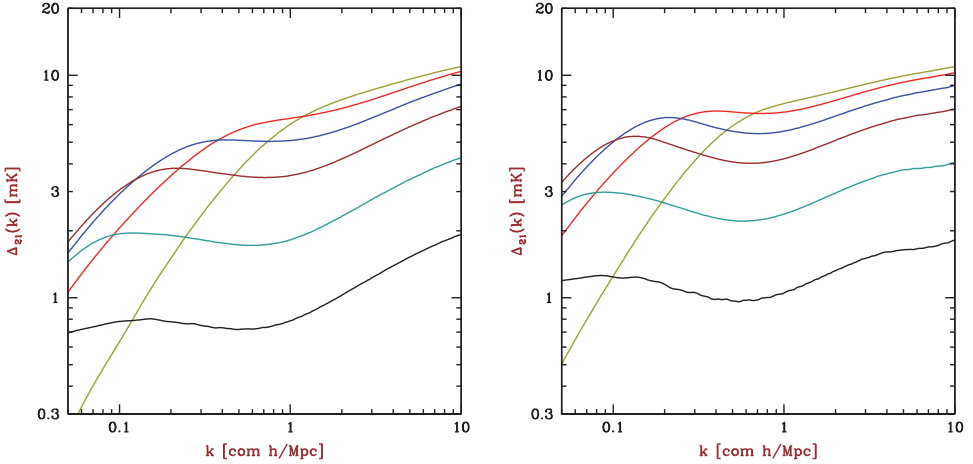


Fig. 15.3. Evolution of the 21-cm power spectrum throughout reionization, for a model that sets the cosmic mean ionized fraction $\bar{x}_i = 98\%$ at $z = 6.5$. Shown are times when $\bar{x}_i = 10\%$, 30% , 50% , 70% , 90% , and 98% (from top to bottom at large k). At the very end of reionization, atomic hydrogen remains only within galaxies (this gas is not included in these plots). The panels show two different possibilities for the masses of galactic halos, assuming a minimum circular velocity for star formation of $V_c = 35$ km/s (left panel) or 100 km/s (right panel). From [8].

likelihood fitting of mock data [8] was done with the analytical model noted above. The computational efficiency of this approach made it possible to employ a flexible six-parameter model that parameterized the uncertainties in the properties of high-redshift galaxies; specifically, the parameters were the coefficients of quadratic polynomial approximations to the redshift evolution of two parameters: the minimum circular velocity of galactic halos, and the overall efficiency of ionizing photon production within galaxies. The conclusion (see Fig. 15.4) was that observations with a first-generation experiment should measure the cosmic ionized fraction to $\sim 1\%$ accuracy at the very end of reionization, and a few percent accuracy around the mid-point of reionization. The mean halo mass hosting the ionizing sources should be measurable to better than 10% accuracy when reionization is $2/3$ of the way through, and to 20% accuracy throughout the central stage of reionization [8]. Recently the semi-numerical code 21CMFAST [9], in a sped-up version that employs some approximations, has been incorporated directly within 21CMMC, a Monte Carlo Markov Chain statistical analysis code. One result derived with this code (see Fig. 15.5) is that combining three observations (at $z = 8, 9$ and 10) of the 21-cm power spectrum will allow upcoming 21-cm arrays to accurately constrain the basic parameters of reionization [10].

15.2. 21-cm signatures of Ly α coupling and LW feedback

As previously discussed, the idea of unusually large fluctuations in the abundance of early galaxies (Sec. 11.2) first made a major impact on studies of cosmic reionization

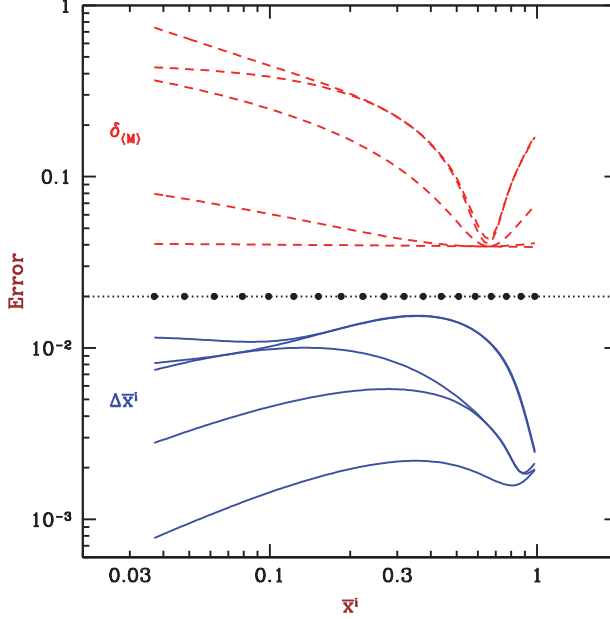


Fig. 15.4. Expected reconstruction errors throughout cosmic reionization, from fitting models to mock data of the 21-cm power spectrum (with the expected errors of a first-generation experiment). The models are based on an analytical model [11, 12] that is in reasonable agreement [8] with numerical simulations of reionization. The x -axis shows the stage of reionization, i.e. the fraction of the IGM that has been reionized ($\bar{x}_i$). Models of varying degrees of flexibility are considered, with 2–6 free parameters (bottom to top in each set of curves). The input model of the mock universe sets the end of reionization (defined as 98% of the IGM being ionized) at $z = 6.5$, with galactic halos assumed to have a minimum circular velocity (Eq. (5.33)) $V_c = 35$ km/s. A horizontal dashed line separates the two areas of the plot that show the expected relative error in the intensity-weighted mean mass of galactic halos (top) and the *absolute* error in the ionized fraction (bottom). Dots on the horizontal line show the values of $\bar{x}_i$ corresponding to the 19 assumed observed redshifts (in the range $z = 6.5 - 12$). From [8].

(Sec. 14.1). The same idea was also key in opening up cosmic dawn, prior to reionization, to interferometric 21-cm observations, by launching the study of fluctuations in the intensity of early cosmic radiation fields. The fact that fluctuations in the galaxy number density cause fluctuations even in the intensity of long-range radiation was first shown, specifically for the Ly α radiation background, by Barkana & Loeb (2005) [13]. The spin temperature of hydrogen atoms in the IGM is coupled to the gas temperature indirectly through the Wouthuysen-Field effect [14, 15], which involves the absorption of Ly α photons (Chap. 12). While it had been previously known [16, 17] that this Ly α coupling likely occurred in the IGM due to Ly α photons emitted by early stars at $z \sim 20-30$, this radiation background had been assumed to be uniform. This intuition was based on the fact that each atom sees Ly α radiation from sources as far away as ~ 300 Mpc. However, it turns out that relatively large, potentially observable, 21-cm fluctuations are generated during the era of initial

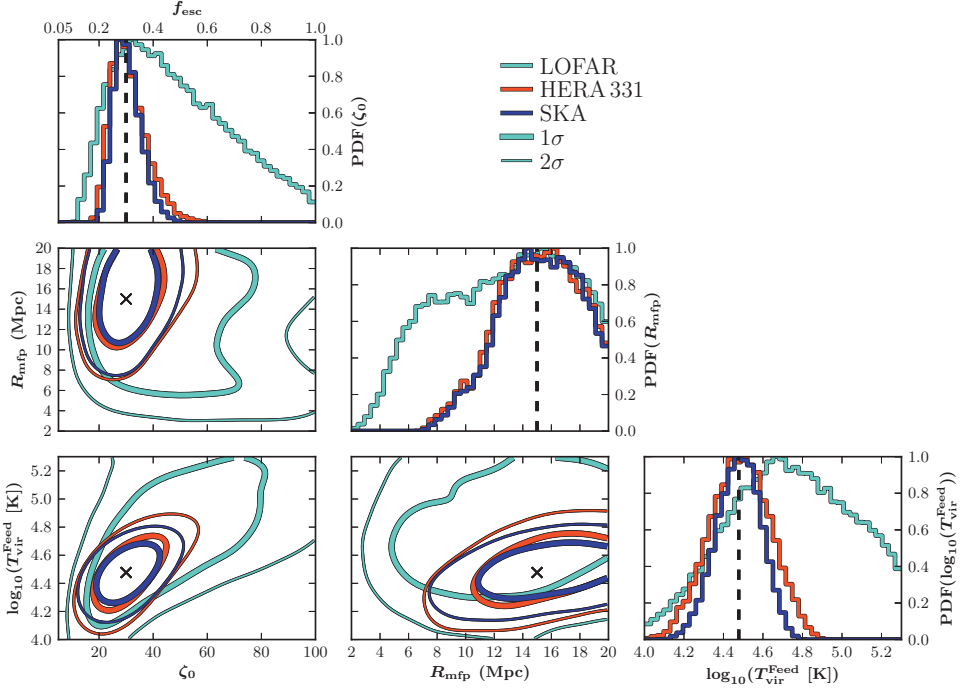


Fig. 15.5. The recovered constraints from 21CMMC on various reionization model parameters from combining three independent ($z = 8, 9$ and 10) 1000 hr observations of the 21 cm power spectrum. Three different telescope arrays are compared: the current LOFAR (turquoise), and the future HERA (red) and SKA phase 1 (blue). Across the diagonal panels, the 1D marginalized PDFs are shown for the recovered reionization parameters [the ionizing efficiency ζ_0 , showing the corresponding escape fraction of ionizing photons f_{esc} on the top; R_{mfp} , the mean free path of ionizing photons within ionized regions; and $\log_{10}(T_{\text{vir}}^{\text{Feed}})$, where $T_{\text{vir}}^{\text{Feed}}$ is the minimum virial temperature of star-forming halos], with the input model parameter value indicated by a vertical dashed line. In the three panels below the diagonal, 2D joint marginalized likelihood contours are shown for various pairs out of the three reionization parameters. The 1σ (thick) and 2σ (thin) contours are shown, with crosses marking the input parameter values. From [10].

$\text{Ly}\alpha$ coupling, for two reasons: fluctuations in the number density of the (highly biased) early galaxies are significant even on scales of order 100 Mpc, and also a significant fraction of the $\text{Ly}\alpha$ flux received by each atom comes from sources at smaller distances. Since relatively few galaxies contribute most of the flux seen at any given point, Poisson fluctuations can be significant as well, producing correlated 21-cm fluctuations (since a single galaxy contributes $\text{Ly}\alpha$ flux to many surrounding points in the IGM). If observed, the $\text{Ly}\alpha$ fluctuation signal would not only constitute the first detection of these early galaxies, but the shape and amplitude of the resulting 21-cm power spectrum would also probe their average properties [13] (Fig. 15.6).

This discovery of $\text{Ly}\alpha$ fluctuations has led to a variety of follow-up work, including more precise analyses of the atomic cascades of Lyman series photons [19, 20].

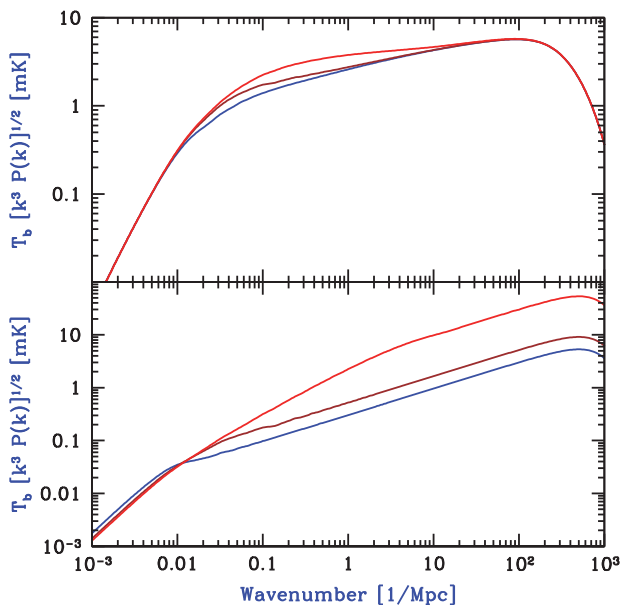


Fig. 15.6. Power spectra of 21-cm brightness fluctuations (in mK units) from Ly α fluctuations, plotted versus (comoving) wavenumber. Shown are two components of the power spectrum that in principle can be separated (in the limit of linear perturbations) based on the line-of-sight anisotropy of the 21-cm fluctuations [18] (Sec. 12.3): $P_{\mu 2}$ (top panel) contains contributions directly from density fluctuations and from the density-induced fluctuations in galaxy density and therefore in Ly α flux, and $P_{un-\delta}$ (bottom panel) is due to Ly α fluctuations from Poisson fluctuations in galaxy numbers. These results are for galaxies formed via atomic cooling in halos at $z = 20$, with a star formation efficiency set to produce the Ly α coupling transition at this redshift. They also assume linear fluctuations, and that the IGM gas cooled adiabatically down to this redshift. Each set of solid curves includes, from bottom to top at $k = 0.1 \text{ Mpc}^{-1}$, stellar radiation emitted up to Ly β , Ly δ , or full Lyman-band emission, all assuming Pop III stars. Note that the results shown here from the first such prediction [13] were later updated (Fig. 15.7).

Also, a significant boost is predicted in the 21-cm power spectrum from Ly α fluctuations due to the repeated scattering of the photons from stars on their way to the hydrogen atoms, out in the wing of the Ly α line [21–23] (Fig. 15.7). The repeated scatterings mean that the Ly α photons do not reach as far (in the fixed time until they redshift into — and then out of — the line), which decreases the overall large-scale smoothing and thus increases the predicted level of 21-cm fluctuations. Moreover, the increased sensitivity to Ly α photons from short distances makes the overall 21-cm power spectrum sensitive to the sizes of H II regions at this very early stage in reionization (Fig. 15.7). Note that in addition to direct stellar emission, Ly α photons are also produced in the IGM from X-ray ionization; however, despite early overestimates [24], the contribution of these Ly α photons in typical models is $\sim 1\%$ compared to stellar Ly α photons [25].

As discussed in Sec. 14.2, LW feedback is an important feedback effect on early galaxies, as it dissociates molecular hydrogen and eventually ends star formation

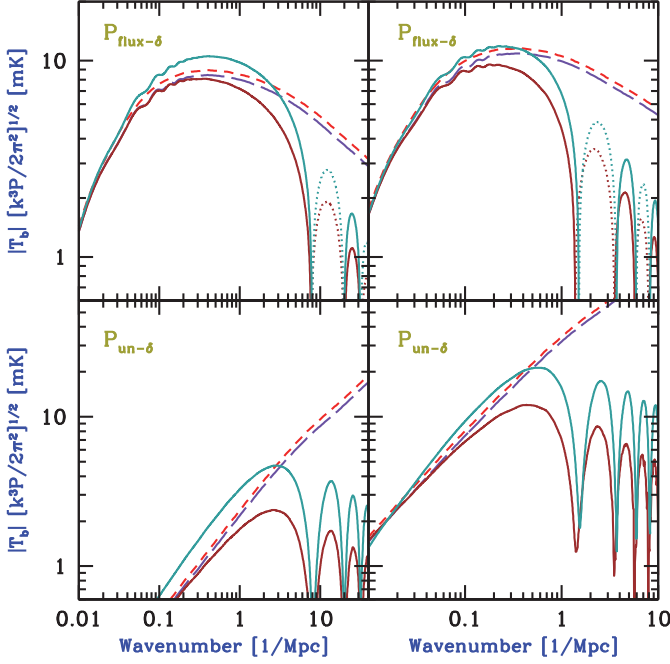


Fig. 15.7. 21-cm power spectrum P (in terms of the brightness temperature fluctuation at wavenumber k) as a function of k . Shown are two components of the power spectrum that in principle can be separated (in the limit of linear perturbations) based on the line-of-sight anisotropy of the 21-cm fluctuations [18] (Sec. 12.3): $P_{\text{flux}-\delta}$ (top panels) contains the contribution of density-induced Ly α fluctuations and $P_{\text{un}-\delta}$ (bottom panels) is due to Ly α fluctuations from Poisson fluctuations in galaxy numbers. Compared here are the earlier result from [13] (including the correction from [19, 20]) (short-dashed curves), the result corrected to use the precise density and temperature power spectra from [26] (long-dashed curves), and from [23] the same calculation with a cutoff due to individual H II regions around galaxies (solid curves, the lower of each pair), and the full calculation (higher solid curve of each pair) which also includes the redistribution of photons due to scattering in the wing of the Ly α line. Two possible examples are shown for galactic halos, where their minimum circular velocity is assumed to be $V_c = 16.5$ km/s (left panels, corresponding to atomic cooling) or $V_c = 35.5$ km/s (right panels, an example of a case where internal feedback makes lower-mass halos inefficient at star formation). Negative portions are shown dotted in absolute value. Note that these results assume the simple case of a fixed H II region size around all galaxies; more realistically, the small-scale ringing seen in this figure may be smoothed out by a scatter in H II region sizes, but the overall shape and the peak of each curve are more robust predictions. From [23].

driven by molecular cooling [27]. Thus, it affects 21-cm fluctuations indirectly by changing the amount and distribution of star formation [28]. The effect becomes particularly striking once the baryon–dark matter streaming velocity (Chap. 13) is included. Assuming that star formation is dominated by $10^6 M_\odot$ halos at very high redshift, the streaming velocity strongly affects them and produces a distinctive BAO signature in the 21-cm fluctuations (Sec. 15.3). Since LW feedback affects star formation in precisely the same halos that are affected by the streaming velocity, the

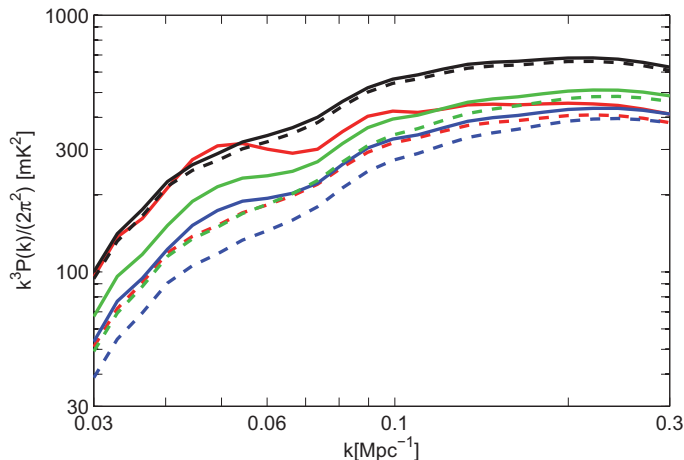


Fig. 15.8. Power spectra of the 21-cm brightness temperature for various strengths of LW feedback: no feedback (red), relatively weak feedback (blue), relatively strong feedback (green) and saturated feedback (i.e. no H_2 molecules; black); each case is shown either with (solid) or without (dashed) the streaming velocity. The weak and strong feedback cases roughly bracket current uncertainties, although recent simulations [30] give some support to the strong case. The results in each case are shown at a time of particularly strong heating fluctuations, a $\Delta z = 3$ earlier (i.e. higher z) than the moment when the cosmic mean 21-cm temperature is zero. The streaming velocity increases and flattens the large-scale power spectrum, and strengthens the BAOs (e.g. at the large-scale peak at $k = 0.05 \text{ Mpc}^{-1}$); this effect (which is wiped out in the limiting case of saturated feedback) is partially suppressed by the LW feedback. This figure from [29] assumed the case of early cosmic heating by a soft X-ray spectrum (Sec. 15.3); in the more likely case of late heating by a hard X-ray spectrum (Sec. 15.4), the combined effect of LW feedback and the streaming velocity would be more difficult to observe with heating fluctuations, but would still be observable during the somewhat earlier era of $\text{Ly}\alpha$ fluctuations.

effectiveness of the feedback has a major effect on 21-cm observations [29] (Fig. 15.8). This is particularly important since there is a substantial uncertainty in the strength of LW feedback on early star formation (although this subject has been explored somewhat with numerical simulations: Sec. 14.2); thus, the prospect that 21-cm observations over a range of redshifts will detect the time evolution of the LW feedback is quite interesting.

15.3. Large 21-cm fluctuations from early cosmic heating

As discussed in detail in Sec. 14.3, until recently it was expected that the universe had been pre-heated well before cosmic reionization. This early heating was thought to be likely due to the high heating efficiency of the soft X-ray spectrum that had been assumed in calculations of cosmic heating. Soft X-rays are absorbed in the neutral IGM over relatively short distances, making heating a local phenomenon that can potentially give rise to large temperature fluctuations in the early IGM. Indeed, when combined with the idea of unusually large fluctuations in the abundance of

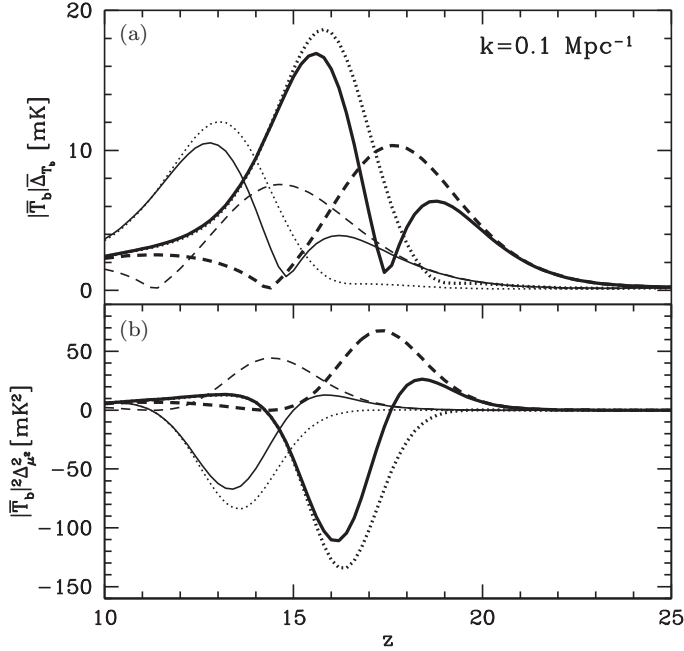


Fig. 15.9. Power spectra of 21-cm brightness fluctuations from temperature fluctuations during cosmic X-ray heating [24]. Shown are the total isotropically-averaged fluctuation (top panel) and the main anisotropic term P_{μ^2} (bottom panel) from the line-of-sight anisotropy of the 21-cm fluctuations [18] (Sec. 12.3). These quantities are shown at a wavenumber $k = 0.1 \text{ Mpc}^{-1}$, including the effects of heating fluctuations only (dotted curves), $\text{Ly}\alpha$ fluctuations only (dashed curves), or both (solid curves). Two models are shown, one corresponding to Pop II stars (thick curves) and the other to Pop III stars (thin curves). Note that this figure from [24] assumed linear fluctuations, early heating by a soft spectrum of X-ray sources, and did not include the boost in the $\text{Ly}\alpha$ fluctuations by a factor of ~ 1.5 (Fig. 15.7) from multiple scattering.

early galaxies (Sec. 11.2), the expectation of large-scale fluctuations in ionization (Sec. 14.1) and in the $\text{Ly}\alpha$ radiation background (Sec. 15.2) can be extended to the X-ray background. The first calculation of heating due to an inhomogeneous X-ray background, by Pritchard & Furlanetto (2007) [24], applied to X-rays a similar method as in the $\text{Ly}\alpha$ case [13]; integrating the heating over time to find the distribution of gas temperatures, the result was the prediction of another era of detectably large 21-cm fluctuations (Fig. 15.9).

As discussed in Sec. 11.3, while numerical simulations are the best, most accurate method for studying early galaxy formation on small scales, they are unable to simultaneously cover large volumes. Simulations that successfully resolve the tiny mini-galaxies that dominated star formation at early times are limited to $\sim 1 \text{ Mpc}$ volumes, and cannot explore the large cosmological scales that might be accessible to 21-cm observations (which are currently limited to low resolution). On the other hand, analytical calculations are limited to linear (plus sometimes weakly non-linear) scales, and thus cannot directly probe the non-linear astrophysics of halo

and star formation. Even if the results of simulations are incorporated within them, analytical approaches assume small fluctuations and linear bias (see Sec. 11.1.1), assumptions that break down in the current context, where the stellar density varies by orders of magnitude on scales of a few Mpc. Even on 100 Mpc scales, fluctuations in the gas temperature are as large as order unity (see below). Thus, linear, analytical calculations can only yield rough estimates, even for large-scale fluctuations.

As a result of these considerations, perhaps the best current method to generate observable 21-cm predictions from the era of early galaxies is with a hybrid, semi-numerical code that combines linear theory and full calculations on large scales with analytical models and the results of numerical simulations on small scales. Such methods have been compared with numerical simulations of reionization [6, 7], and have also been used to predict the effect of the streaming velocity on high-redshift galaxy formation [31, 32]. Figure 15.10 shows a prediction of the 21-cm signatures of X-ray heating made with the semi-numerical code 21CMFAST [33]. The light-cone slices show the progression through cosmic 21-cm history: collisional decoupling during the dark ages (black, far-right region), $\text{Ly}\alpha$ coupling (black to yellow transition), X-ray heating (yellow to blue), and reionization (blue to black).

In the case of soft X-ray heating sources, heating fluctuations are the largest, most promising source of pre-reionization 21-cm fluctuations, but even in this case there remains a large uncertainty in predicting the signal. The redshift at which this signal peaks depends on the overall efficiency of X-ray production, with higher efficiency leading to an earlier cosmic heating era. This uncertainty is not too problematic since planned observations will cover a wide redshift range and find the signal if it is there. Given the correct redshift, the strength of the signal still depends on the typical mass of the galactic halos that hosted these sources. The more massive the halos, the more highly biased (clustered) they are expected to have been, thus producing a larger 21-cm fluctuation signal. However, the baryon–dark matter streaming velocity (Chap. 13) greatly cuts down this uncertainty, as it boosts the expected signal from low-mass halos nearly to the same level as that from high-mass halos. Observational predictions that include the streaming velocity were achieved with a semi-numerical method [34].

This approach built upon previous semi-numerical methods used for high-redshift galaxy formation [9, 31, 32]. It used the known statistical properties of the initial density and velocity perturbations to generate a realistic sample universe on large, linear scales. This was followed by a calculation of the stellar content of each pixel on the grid using a model [35] previously developed to describe the streaming velocity effect on galaxy formation; this includes analytical models as well as fits to the results of small-scale numerical simulations. Like other semi-numerical codes, it assumed standard initial perturbations (e.g. from a period of inflation), where the density and velocity components are Gaussian random fields.

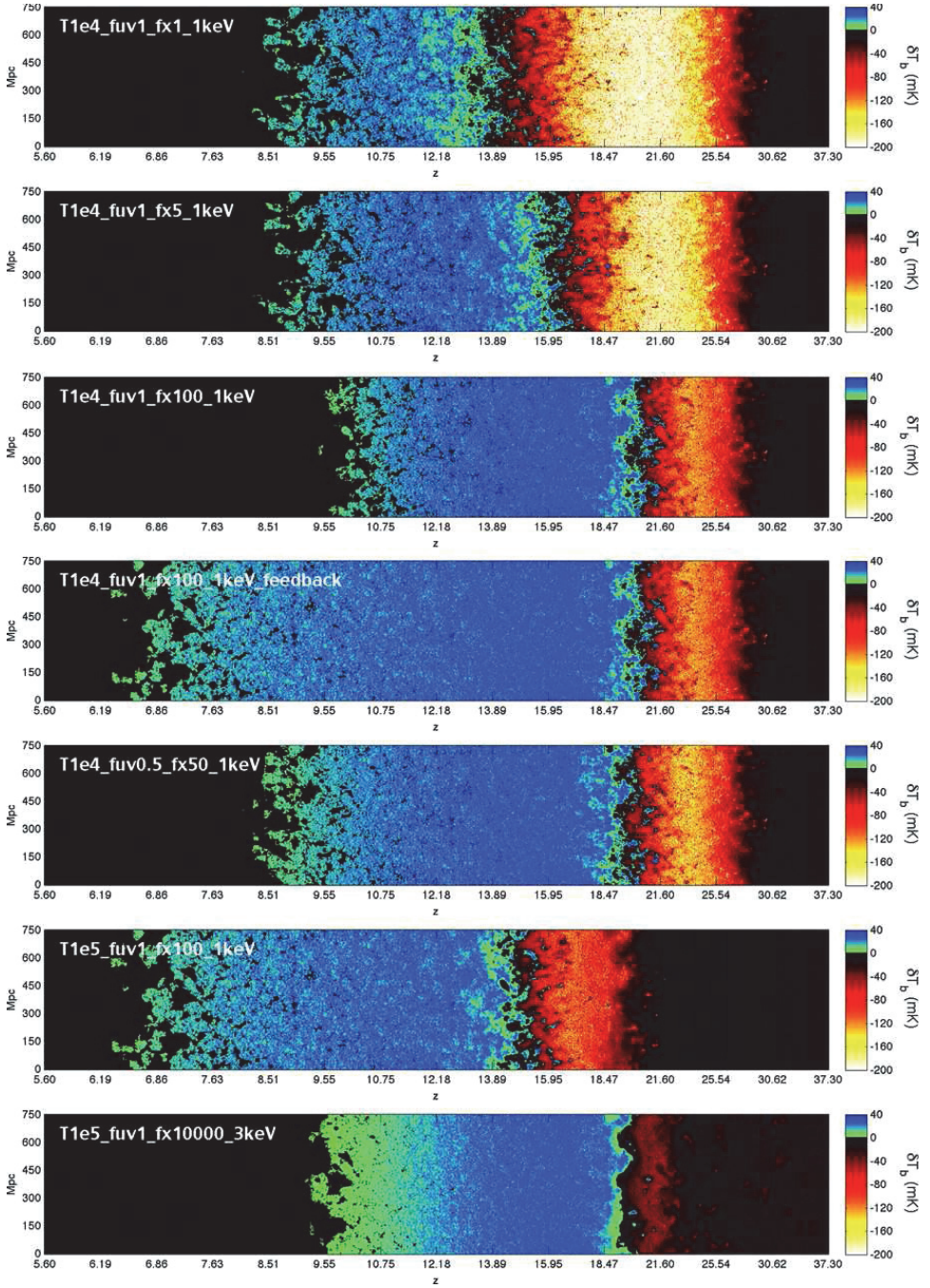


Fig. 15.10. (figure on facing page) Slices through the predicted 21 cm signal for models calculated with the semi-numerical code 21CMFAST. The slices show the evolution of the 21-cm brightness temperature with distance along the light cone, with the redshift indicated on the x -axis, and the y -axis showing spatial structure at each redshift. In the model name, T indicates the minimum assumed virial temperature of galactic halos (10^4 K corresponds to atomic cooling), fuv and fx parameterize the ionizing and X-ray efficiency, respectively, and the final number indicates the mean X-ray photon energy (“1 keV” indicates a soft power-law starting at 0.3 keV, with a mean photon energy of 0.9 keV; these quantities are 3 times larger for the “3 keV” case). These models assume heating via soft X-rays, except for the extreme (bottom-most) model in which very intense X-rays dominate reionization (not just heating). From [33].

Velocities are coherent on larger scales than the density, due to the extra factor of $1/k$ in the velocity from the continuity equation that relates the two fields. This is clearly apparent in the example shown in Fig. 15.11 of a thin slice of a simulated volume. The density field fluctuates on relatively small scales, while the velocity field shows a larger-scale cosmic web, with coherent structure on scales of order 100 Mpc. This means that the largest scales will be dominated by the pattern due to the velocity effect, as long as the streaming velocity significantly affects star formation.

The resulting distribution of stellar density at $z = 20$ is also shown in Fig. 15.11. Note the large biasing (amplification of fluctuations) of the stars: density fluctuations ranging up to $\pm 50\%$ yield (without including the streaming velocity) a field of stellar density that varies by over a factor of 20 (when both fields are smoothed on a 3 Mpc scale). The velocity effect produces a more prominent cosmic web on large scales, marked by large coherent regions that have a low density of stars, separated by ribbons or filaments of high star formation. The effect is much more striking at higher redshifts (Fig. 15.12), and it thus substantially alters the feedback environment of the very first generations of stars. The various types of radiation that produce feedback spread out to a considerable distance from each source, but this distance is typically not as large as the span of the velocity-induced features. This means that regions of low velocity (and thus high star formation) experience radiative feedback substantially earlier than regions of high velocity (low star formation). Thus, the substantial effect of the velocities on early star formation makes early feedback much more inhomogeneous than previously thought.

Observationally, these degree-scale fluctuations affect various cosmic radiation backgrounds, and in particular the history of 21-cm emission and absorption. As noted above, in the presence of soft X-ray heating sources, the heating fluctuations produce the largest pre-reionization 21-cm fluctuations, typically from sometime after the Ly α coupling has mostly saturated. As for the LW flux, here we consider the case of negligible LW feedback (as was assumed in Figs. 15.11 and 15.12), but below we bracket the effect of the LW flux by also considering the opposite limiting case where the LW transition has already saturated (i.e. completely destroyed hydrogen

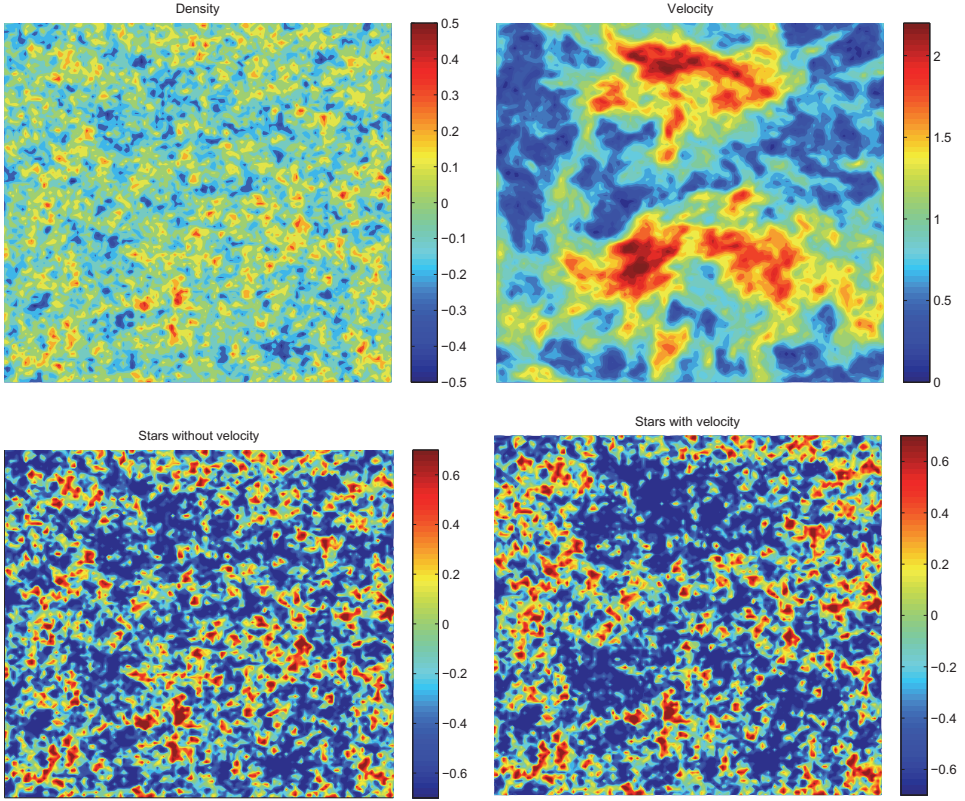


Fig. 15.11. Effect of the streaming velocity on the number density of stars at redshift 20. The large-scale density (top left panel) and velocity (top right panel) fields are shown on the top. For the density field, the fractional perturbation relative to the mean is shown, at $z = 20$; for the velocity field, the magnitude of the relative motion in units of the root-mean-square value is shown (the map is independent of redshift in these relative units). For the same slice, the traditional calculation (lower left panel), which includes the effect of density only, is compared to the new prediction (lower right panel), which includes the effect of the same density field plus that of the streaming velocity. The colors in the bottom panels correspond to the logarithm (base 10) of the gas fraction in units of its cosmic mean value in each case. The panels all show a 3 Mpc thick slice (the pixel size of the grid in the semi-numerical code) from a simulated volume 384 Mpc on a side (based on [34], but taken from a different box from the one shown in the figures in [34], i.e. for a different set of random initial conditions).

molecules); the effect of various strengths of LW feedback was discussed in more detail in Sec. 15.2.

Figure 15.13 shows the gas temperature distribution at $z = 20$, assumed to be at the heating transition, i.e. when the mean H I gas temperature was equal to that of the CMB. Regions where the gas moved rapidly with respect to the dark matter (dark red regions, top right panel of Fig. 15.11) produced fewer stars (dark blue regions, bottom right panel of Fig. 15.11) and thus a lower X-ray intensity, leaving large regions with gas that is still colder than the CMB by a factor of several (dark

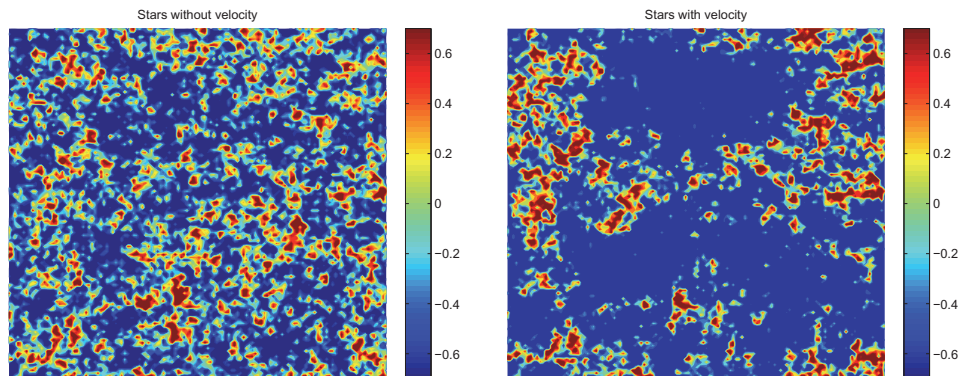


Fig. 15.12. Effect of the streaming velocity on the number density of stars at redshift 40. For the same slice as in Fig. 15.11, we compare the traditional calculation (left panel), which includes the effect of density only, to the new prediction (right panel), which includes the effect of the same density field plus that of the streaming velocity. The colors correspond to the logarithm of the gas fraction in units of its cosmic mean value in each case. The color scale spans the same range as in Fig. 15.11 for easy comparison.

blue regions, top right panel of Fig. 15.13). The spatial reach of X-rays results in a gas temperature distribution that is smoother than the distribution of stars, and this brings out the effect of large-scale fluctuations and thus highlights the contrast between the effect of density and velocity fluctuations.

During the heating transition (Sec. 14.3), the 21-cm brightness temperature (shown in the bottom panels of Fig. 15.13) mainly measures the gas (kinetic) temperature T_K , although it is also proportional to the gas density (and to the square root of $1 + z$). The form of the dependence, $T_b \propto 1 - T_{\text{CMB}}/T_K$, makes the 21-cm intensity more sensitive to cold gas than to hot gas (relative to the CMB temperature). Thus, the large voids in star formation produced by a high streaming velocity lead to prominent 21-cm absorption (dark blue regions, bottom right panel of Fig. 15.13) seen on top of the pattern from the effect of density fluctuations. These deep 21-cm cold spots are a major observable signature of the effect of the streaming velocity on early galaxies.

While Fig. 15.13 illustrates the detailed pattern that the streaming velocity imprints on the 21-cm intensity distribution, upcoming experiments are expected to yield noisy maps that likely must be analyzed statistically. Figure 15.14 shows the predicted effect on the power spectrum of the fluctuations in 21-cm intensity [34]. The velocities enhance large-scale fluctuations (blue solid curve compared with red dotted), leading to a flatter power spectrum with prominent baryon acoustic oscillations (reflecting the BAO signature in Fig. 13.1). The signal is potentially observable with a redshift 20 version of current instruments (green dashed curve). If there is complete LW feedback (solid purple curve), then the small galaxies that rely on molecular-hydrogen cooling are unable to form; the larger galaxies that dominate in that case are almost unaffected by the streaming velocity, so the 21-cm

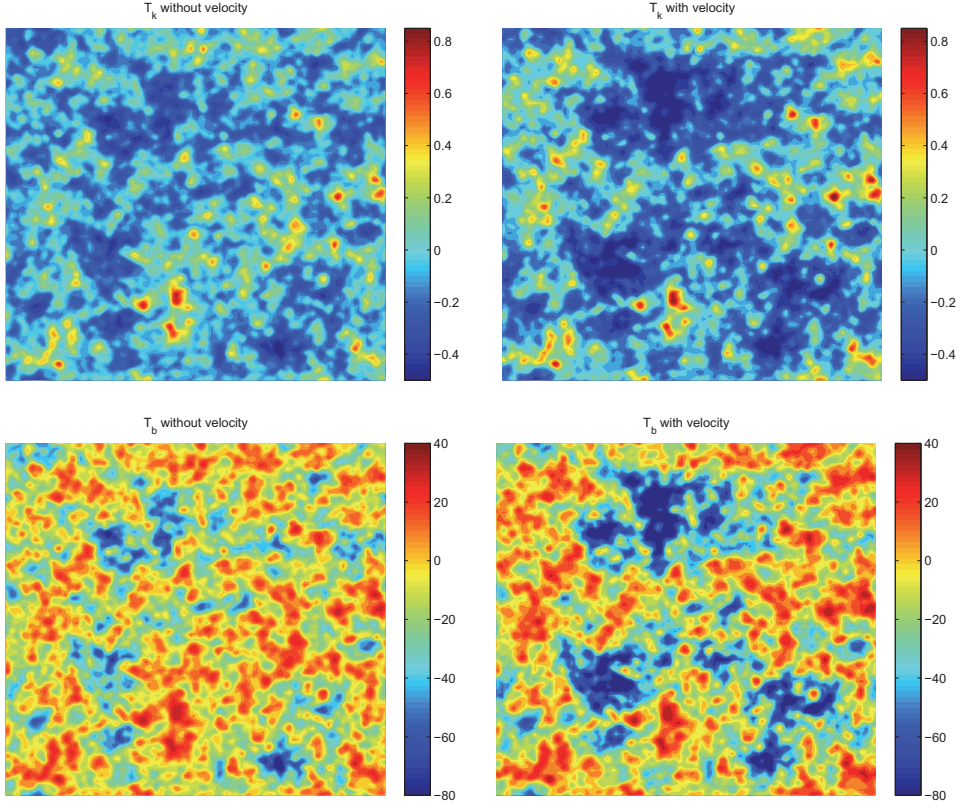


Fig. 15.13. Effect of the streaming velocity on the gas temperature T_k and on the 21-cm brightness temperature T_b at redshift 20. For the same slice as in Fig. 15.11, we compare the traditional calculations (left-hand panels), which include the effect of density only, to the new predictions (right-hand panels), which include the effect of density and streaming velocity. The colors in the top panels correspond to the logarithm of the gas (kinetic) temperature in units of the CMB temperature at $z = 20$. The colors in the bottom panels correspond to the 21-cm brightness temperature in millikelvin units. Note that the observed wavelength of this 21-cm radiation is redshifted by the expansion of the universe to 4.4 meters (corresponding to a frequency of 68 MHz).

power spectrum reverts to the density-dominated shape (compare the solid purple and red dotted curves), but it becomes even higher since more massive galactic halos are even more strongly biased.

Thus, regardless of the strength of the LW feedback (or other negative feedback effects on small galaxies), the 21-cm power spectrum at the peak of the heating transition should feature large fluctuations on observable scales. Beyond just detection of the signal, only a mild additional accuracy is necessary in order to determine whether feedback has suppressed star formation in the smallest halos. If it has not, then the velocity effect produces strong BAOs on top of a flattened power spectrum, in particular raising it by a factor of 4 on large scales ($k = 0.05 \text{ Mpc}^{-1}$, wavelength 130 Mpc, observed angle $2/3$ of a degree) where the experimental sensitivity is

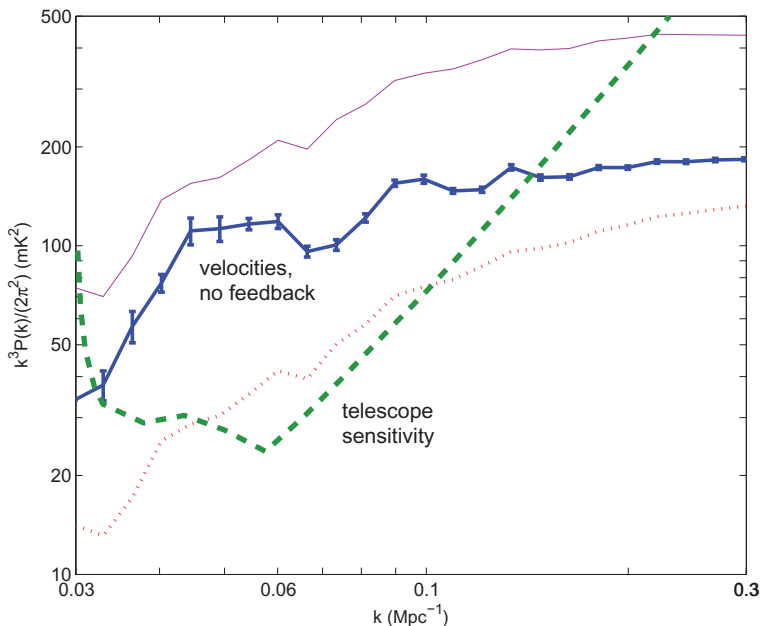


Fig. 15.14. Signature of the streaming velocity in the 21-cm power spectrum, at the peak of the X-ray heating transition. The prediction is shown including the streaming velocity effect (blue solid curve) or with the effect of density only (red dotted curve), both for the case of a late LW transition for which the LW feedback is still negligible at the heating transition. These predictions are compared to the projected 1σ telescope sensitivity (green dashed curve) based on a 1000-hour observation with an instrument like the Murchison Wide-field Array or the Low Frequency Array but designed to operate at 50–100 MHz [1], including an estimated degradation factor due to foreground removal [36]; this sensitivity is defined as the signal that would yield a measurement with a signal-to-noise ratio of unity in each k bin of size $\Delta k = 0.5k$ averaged over an 8 MHz frequency band (where only thermal noise is included). Future experiments like the Square Kilometer Array should reach a better sensitivity by more than an order of magnitude [1]. To allow for the possibility of feedback, the prediction is also shown in the opposite limit of maximum feedback, i.e. an early LW transition that has already saturated (purple solid curve). In this plot, the heating transition has been fixed at $z = 20$ for easy comparison among the various cases. Error bars on the main prediction curve indicate the 1σ sample variance in one simulation box. From [34].

optimal. If this characteristic shape is observed it would confirm that million mass halos dominated galaxy formation at this early epoch.

While Fig. 15.14 considers a single redshift, similar observations over the full $\Delta z \sim 6$ redshift range of significant heating fluctuations could actually detect the slow advance of the LW feedback process, during which the power spectrum is predicted to continuously change shape, gradually steepening as the BAO signature weakens towards low redshift (see Fig. 15.8 in Sec. 15.2). This is all the case if the Universe was heated by soft X-rays. If it was heated by hard X-rays (see the next section), then the heating peak is largely erased, but similar effects of the streaming velocity are expected on the 21-cm signal during the $z \sim 25$ fluctuation peak from the Lyman- α coupling transition (Sec. 15.2).

15.4. Late heating and reionization

As discussed in Sec. 14.3, it was recently realized that the hard X-ray spectrum characteristic of X-ray binaries, the most plausible source of early cosmic heating, is predicted to have produced a relatively late heating, possibly encroaching on the reionization era. The effect of this on the global 21-cm signal is discussed in Sec. 15.5. Here we discuss the key consequences for 21-cm fluctuations.

A major effect of X-ray heating by a hard spectrum is the suppression of 21-cm fluctuations due to heating. Under the previously assumed soft spectra, the short typical distance traveled by the X-ray photons was found to produce large fluctuations in the gas temperature and thus in the 21-cm intensity around the time of the heating transition, regardless of when this transition occurred [24, 34, 37] (Sec. 15.3). However, the larger source distances associated with a hard spectrum lead to a much more uniform heating, with correspondingly low temperature fluctuations even around the time of the heating transition, when the 21-cm intensity is quite sensitive to the gas temperature. This trend is strengthened by late heating, as it occurs at a time when the heating sources are no longer as rare and strongly biased as they would be in the case of an earlier heating era. Thus, heating with a hard X-ray spectrum is predicted to produce a new signature in the 21-cm fluctuation signal: a deep *minimum* during reionization [38]. This results from the low level of gas temperature fluctuations in combination with a suppression of the 21-cm impact of other types of fluctuations (i.e. in density and ionization); in particular, right at the heating transition, the cosmic mean 21-cm intensity is (very nearly) zero, and thus all fluctuations other than those in the gas temperature disappear (to linear order) from the 21-cm sky.

This effect is visually apparent in simulated maps (Fig. 15.15). In upcoming observations, it is likely to be apparent in the measured 21-cm power spectrum (Fig. 15.16). Depending on the parameters, the deep minimum (reaching below 1 mK) may occur at any time during reionization, but is likely to occur before its mid-point. Previously, the fluctuation signal was expected to lie within a narrow, well-defined range, allowing for a relatively straight-forward interpretation of the data in terms of the progress of reionization; the possibility of a hard X-ray spectrum, however, introduces a variety of possibilities, making it likely that modeling of the 21-cm data will involve an analysis of the interplay of heating and reionization.

If a sufficient sensitivity level can be achieved, a low minimum in the 21-cm power spectrum during reionization would be a clear signature of late heating due to a hard X-ray spectrum. Indeed, a clear observational indication that this feature corresponds to a cosmic milestone is that the minima at all $k > 0.5 \text{ Mpc}^{-1}$ should occur at essentially the same redshift (namely the true redshift of the heating transition); lower wavenumbers correspond to larger scales than the typical X-ray mean free path, leading to a more complicated evolution and to minima delayed to lower redshifts (see also Fig. 16.1). More generally, observations of the 21-cm power

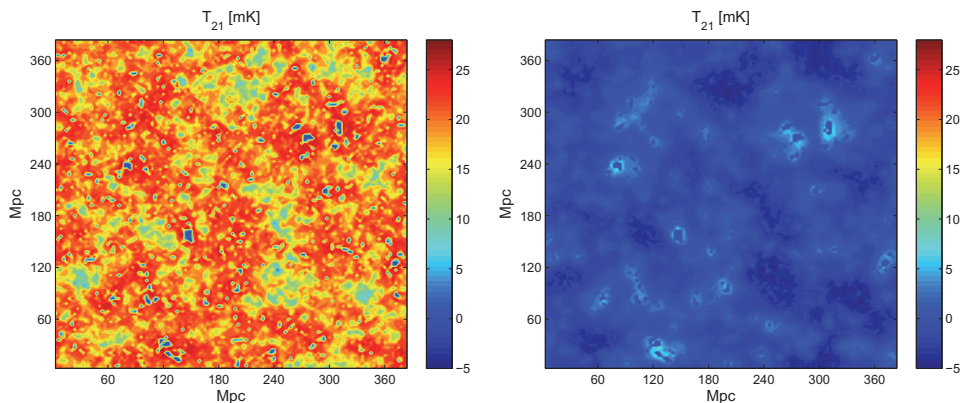


Fig. 15.15. Example of a predicted 21-cm map from a semi-numerical code, at $z = 12.1$, comparing the case of heating sources with a hard X-ray spectrum (right panel) and the previously-assumed soft spectrum (left panel), shown on a common scale. For the hard spectrum, this redshift corresponds to the cosmic heating transition. In this comparison, both cases have the same underlying distribution of star formation at a given redshift, so they have the same ionized patches (at an early stage of reionization, when 14% of the IGM has been reionized) and a similar distribution pattern of gas temperature and of 21-cm temperature. However, the difference is visually striking, in that the map for the hard spectrum is strongly suppressed in terms of both the typical value of T_b and the typical size of its fluctuations. From [39].

spectrum over a broad range of wavenumbers will clearly probe the X-ray spectrum of the sources of cosmic heating [38, 39, 41, 42].

Beyond reionization, heating by high-energy X-rays removes the previously expected signal from an early heating transition (Sec. 15.3) at $z \sim 15 - 20$, but leaves in place the similar $z \sim 20 - 25$ signal from the Lyman- α coupling transition that is likely detectable with the Square Kilometre Array (Sec. 15.2); actually, in this case the Ly α peak is stronger and more extended in redshift, since it is not cut off by early heating as in the case of soft X-rays [39]. It could also affect other observations of high-redshift galaxies. For example, since late heating implies weak photoheating feedback during the cosmic heating era, low-mass halos may continue to produce copious stars in each region right up to its local reionization; note though that internal feedback (arising from supernovae or mini-quasars) could still limit star formation in small halos.

15.5. The global 21-cm spectrum

This section thus far has focused on 21-cm fluctuations, and in particular the 21-cm power spectrum. The power spectrum encodes a lot of information about the various sources of 21-cm fluctuations, and it is a rich dataset consisting of an entire function of wavenumber at each redshift, or potentially even much more than that due to the line-of-sight anisotropy (Sec. 12.3). This information can hopefully be extracted from data obtained with radio interferometers, after dealing with the

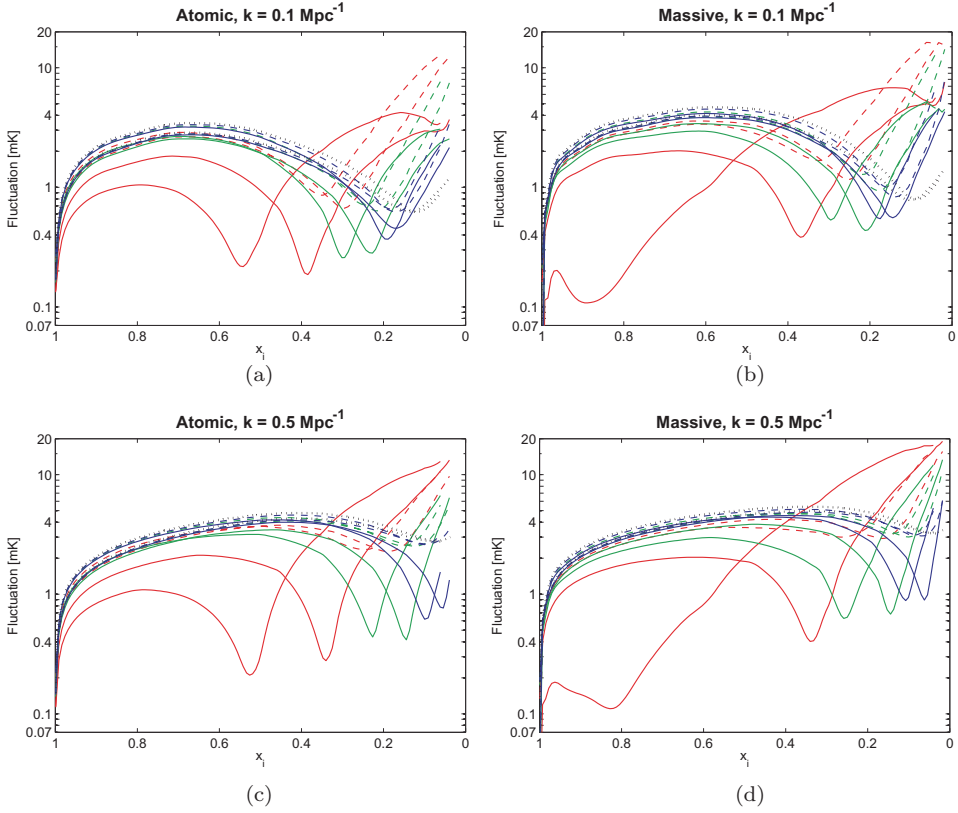


Fig. 15.16. The fluctuation level of the 21-cm brightness temperature is shown versus the ionized (mass) fraction of the universe x_i (starting on the right from $z = 15$). We compare results obtained with a hard X-ray binary spectrum [40] (solid curves) to those with the previously-adopted soft spectrum (dashed curves), and show the commonly-assumed saturated heating case for reference (black dotted curves). The curves show various cases, in order to give a reasonable idea of the range of parameter space given current uncertainties. Thus, the best guess for the X-ray efficiency (green curves) is shown along with an efficiency lower (red curves) or higher (blue curves) by a factor of $\sqrt{10}$, each with either early or late reionization (given current uncertainties about its timing: see Sec. 14.1). The fluctuation is shown at a wavenumber $k = 0.1 \text{ Mpc}^{-1}$ (top panels) or $k = 0.5 \text{ Mpc}^{-1}$ (bottom panels), for two possible cases of galactic halos, either a minimum halo mass set by atomic cooling (left panels) or halos that are ten times more massive (right panels). The lower k value roughly tracks large-scale fluctuations (heating early on, and ionized bubbles later), while the higher k value corresponds to a smaller scale (though one that can still be measured accurately with current experiments) and thus tracks more closely the evolution of density fluctuations. To illustrate the effect of the X-ray spectrum on the results, consider the fluctuation level at $k = 0.5 \text{ Mpc}^{-1}$ at the mid-point of reionization (i.e. $x_i = 0.5$); the parameter space explored here gives a possible range of 3.6–4.9 mK for the soft spectrum, while the hard spectrum gives a much broader range of 0.3–4.4 mK. Note also that the latter values are typically much lower than the often-assumed limit of saturated heating (which gives a corresponding range of 4.1–5.1 mK). From [38].

expected thermal noise and sample variance, foreground residuals, and artifacts of the imperfectly-known responses of the radio antennae and receivers.

A very different approach is to measure the total sky spectrum and detect the redshift evolution of the global, cosmic mean 21-cm intensity. A global experiment requires a simple, relatively cheap setup (an all-sky antenna) compared to the fluctuation experiments, and the total sky naturally yields a higher signal-to-noise ratio and a spectrally smoother foreground than found in small patches (which are the basic units of the fluctuation experiments). In order to make success more likely, observations can focus on constraining sharp frequency features, without attempting to measure the absolute cosmological 21-cm emission level (which is much harder). During reionization, there should be a decrease in the global 21-cm emission due to the overall disappearance of atomic hydrogen (Sec. 14.1). This global step, while not sudden, is still expected to be fairly sharp in frequency. At higher redshifts, a sharp decrease towards negative brightness temperature should occur due to the rise of the first stars as a result of Ly α coupling of the cold IGM (Sec. 14.2), followed by a sharp rise up to positive values due to cosmic heating (Sec. 14.3). Thus, a detection of the global signal would trace the overall cosmic history of the first stars through their effect on 21-cm emission (Fig. 15.17). Maximum-likelihood analyses of data

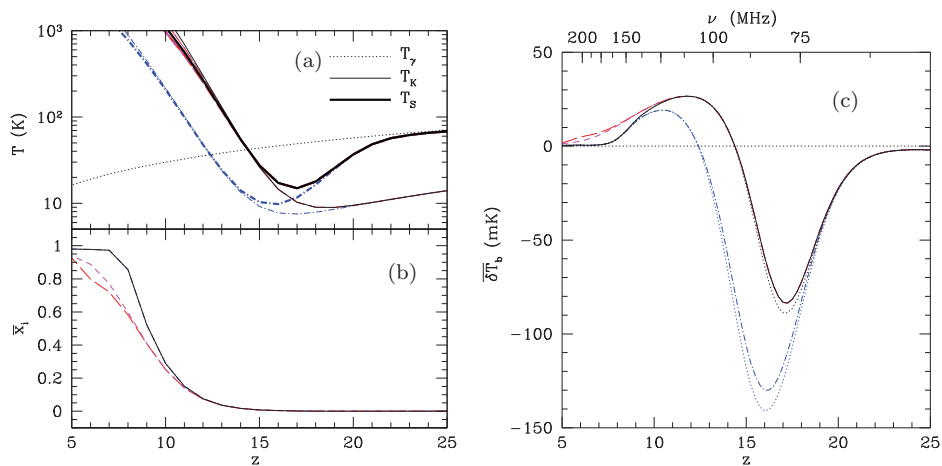


Fig. 15.17. Examples of predicted global 21-cm histories, showing how they reflect the cosmic history of star formation and its various effects on the IGM. A range of parameters are shown in order to reflect a reasonable range of uncertainty: the best-guess X-ray efficiency (solid curves), a lower efficiency by a factor of 5 (dot-dashed curves), and the addition of two possible models for photoheating feedback (short- and long-dashed curves). Panel (a) shows the CMB (T_γ), gas kinetic (T_K) and spin (T_S) temperatures (dotted, thin, and thick solid curves, respectively). Panel (b) shows the progress of reionization, in terms of the cosmic mean ionized fraction $\bar{x}_i$. Panel (c) shows the resulting global mean 21-cm brightness temperature measured with respect to the CMB; in this panel, the two dotted lines show T_b if shock heating is ignored. Note that this panel shows the observed frequency on top in addition to the redshift on the bottom. All models here assume Pop II stars and a soft X-ray spectrum of heating sources. From [45].

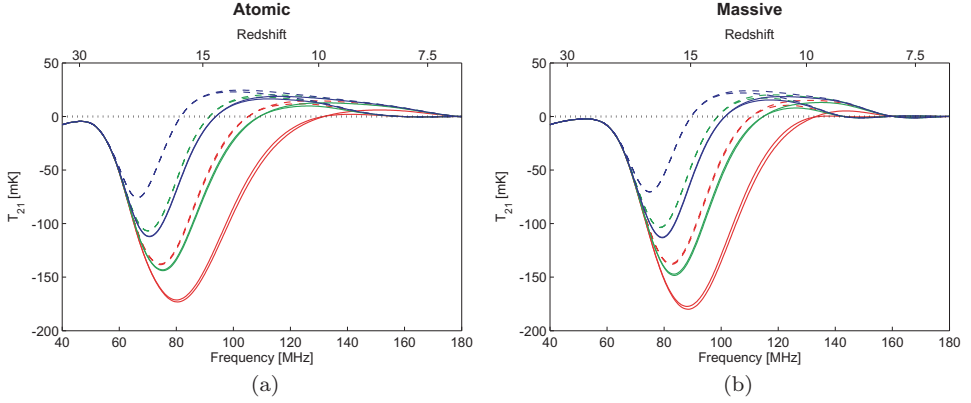


Fig. 15.18. The effect of late cosmic heating on the global 21-cm spectrum. The cosmic mean 21-cm brightness temperature (T_{21}) relative to the CMB is shown versus observed frequency (with the redshift indicated on top), for the hard X-ray binary spectrum [40] (solid curves) and for the previously-adopted soft spectrum (dashed curves); note also the fiducial dotted line at $T_{21} = 0$. Various cases are shown, in order to give a reasonable idea of the range of parameter space given current uncertainties; the notation matches that in Fig. 15.16. From [38].

fitting show that global 21-cm measurements during cosmic reionization should be able to detect a wide range of realistic models and measure the main features of the reionization history while constraining the key properties of the ionizing sources; this is true in analyses (that assumed the saturated heating limit) using a flexible toy model [43] or a Λ CDM-based model [44], though the results are rather sensitive to assumptions on just how difficult it will be to remove the effect of the foregrounds.

If X-ray binaries with a hard spectrum produce late heating (Sec. 14.3 and Sec. 15.4), this will have a particularly important effect on the global 21-cm signal. The effect of late heating is to give the cosmic gas more time to cool adiabatically to well below the CMB temperature, thus producing mean 21-cm absorption that reaches a maximum depth in the range -110 to -180 mK at $z \sim 15 - 19$ (Fig. 15.18). This may make it easier for experiments to detect the global 21-cm spectrum from before reionization and thus probe the corresponding early galaxies. Global experiments are most sensitive to the frequency derivative of the 21-cm brightness temperature; late heating extends the steep portion of the spectrum to higher frequencies, moving the maximum positive derivative to a $\sim 10\%$ higher frequency (where the foregrounds are significantly weaker) while also changing the value of this maximum derivative by $\pm 10\%$. On the other hand, at lower redshift, late heating significantly suppresses the global step from reionization, which suggests that global 21-cm experiments should focus instead on the earlier eras of $\text{Ly}\alpha$ coupling and cosmic heating.

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Chapter 16

Summary and Conclusions

The study of the first stars, galaxies, and black holes, and their effect on the 21-cm sky, is entering a critical stage. While this subject has been developing theoretically for several decades, including a great acceleration in recent years, observationally this field is in its infancy. Thus, we are about to experience that pinnacle of excitement that comes with the first clash of a scientific theory with experimental data. In such a collision of theoretical expectations with reality, there are several possible outcomes. The predictions can be perfectly verified, an outcome that will make the successful theorists gleeful and proud, but at the same time will be quite boring. At the other extreme, the predictions can fail completely, making the theorists a laughing-stock, but revealing previously unexpected cosmic events, which makes this possibility the most exciting one. Neither of these extreme possibilities is expected in the case of 21-cm cosmology. The sheer magnitude of the uncertainty about high-redshift astrophysics makes the first possibility unlikely, even in the absence of exotic cosmic events such as dark matter decay. On the other hand, complete failure is made unlikely by the fact that the theory is grounded in solid atomic physics as well as models of galaxy formation that are significantly constrained by observations of the current Universe, at one end, and the CMB at the other (initial condition) end. Thus, the most likely outcome is an intermediate one, where the overall framework of theoretical expectations will be confirmed, but with some, hopefully interesting and significant, surprises, such as an unexpected, new class of astrophysical sources (which will be noticed if it dominated one of the types of radiation that drove the 21-cm emission). Regardless of the precise outcome, it is likely that once a clear detection of the 21-cm signal from early cosmic history is achieved, the field will get a big boost, analogous to the development of CMB observations and theory after the first detection of CMB temperature fluctuations by the COBE satellite [1]. This breakthrough moment for 21-cm cosmology will hopefully occur within the next few years, and will be followed up with confirmations and more detailed measurements soon afterwards.

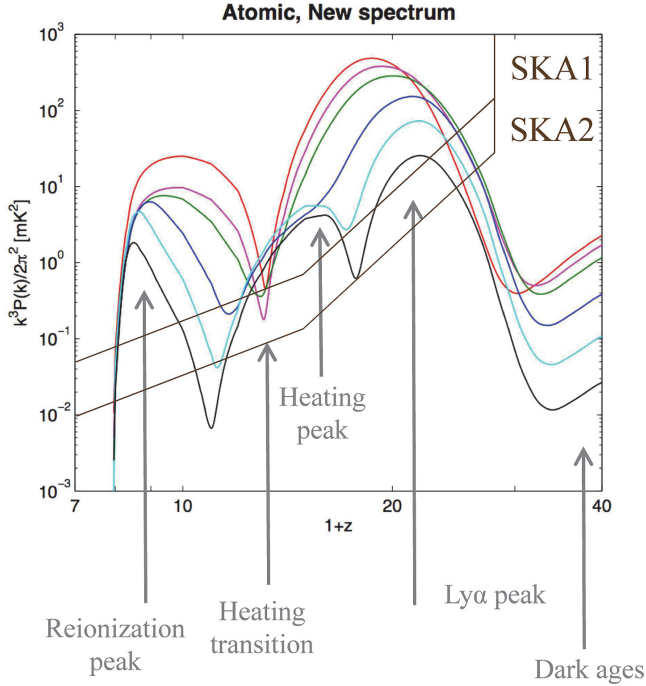


Fig. 16.1. A summary view of the rich complexity of even just the isotropically-averaged 21-cm power spectrum, shown via the evolution with redshift of the squared 21-cm fluctuation at various wavenumbers. Going from small to large scales, shown are $k = 1 \text{ Mpc}^{-1}$ (red), $k = 0.5 \text{ Mpc}^{-1}$ (magenta), $k = 0.3 \text{ Mpc}^{-1}$ (green), $k = 0.1 \text{ Mpc}^{-1}$ (blue), $k = 0.05 \text{ Mpc}^{-1}$ (cyan), and $k = 0.03 \text{ Mpc}^{-1}$ (black). The particular model shown here assumes cosmic heating by a hard X-ray spectrum (Sec. 14.3 and Sec. 15.4), and that stars form in all halos in which the gas can cool via atomic cooling. Also shown is the approximate observational thermal noise power spectrum expected for the SKA phase 1 and phase 2 (at $k = 0.1 \text{ Mpc}^{-1}$) [4]. From [2], with added labels and observational sensitivities.

A great wealth of data is potentially available in 21-cm cosmology (Chap. 14 and Chap. 15). Even just the isotropically-averaged 21-cm power spectrum, measured as a function of wavenumber and redshift, is a rich data set that probes many details of the various cosmological and astrophysical sources of 21-cm fluctuations (see Fig. 16.1). A number of cosmic events leave clear signatures in the power spectrum, but the redshifts of the associated features (such as the peaks) vary with scale, since several different sources of 21-cm fluctuations contribute at any given time, and these sources differ in their scale dependence. In the model shown in Fig. 16.1, for which reionization ends at $z \sim 7$, the reionization peak of fluctuations occurs in the range $z = 7.5 - 9$ depending on wavenumber. While the uncertainties are still large, it now seems that the IGM was most likely heated by X-ray sources with a hard spectrum (Sec. 14.3 and Sec. 15.4), a possibility not considered until recently; in this case, the cosmic heating transition produces a clear minimum on small scales, but a weak heating peak remains on the largest scales that are larger

than the typical distance traveled even by hard X-rays. Continuing with Fig. 16.1, the Ly α peak occurs in this example at $z = 18 - 20$, and (generally in the case of late heating) it is both the strongest and highest-redshift signal from the first stars (In the case of a soft X-ray spectrum, the heating peak is somewhat higher than the Ly α peak [2]). We note that additional theoretical uncertainties result from the complexity of the astrophysics during early times, including major, spatially inhomogeneous transitions in the basic character of star formation expected due to various types of stellar feedback such as supernova outflows, LW radiation, and metal enrichment. The dark ages, during which 21-cm emission was not significantly affected by astrophysical sources and serves as a purely cosmological probe, appear in this case at $z > 30$; at this point the predicted fluctuation signal is quite low, and since the galactic foreground increases rapidly with redshift (with the brightness temperature of the sky $\propto (1+z)^{2.6}$ [3]), observations of this era lie in the somewhat distant future.

Actually measuring a data set like that shown in Fig. 16.1 would obviously constitute an amazing advance in our understanding of cosmic history. However, it is important to also look for robust, model-independent signatures that can convincingly confirm and complement the results obtained from fitting parameterized models to the (angle-averaged) 21-cm power spectrum. This is particularly needed in a field looking to probe a new, unexplored regime of cosmic history, with few known options for other types of complementary observations. Luckily, the field of 21-cm cosmology has turned out to be a very rich one. For example, the line-of-sight anisotropy of the power spectrum (Sec. 12.3) is potentially an immensely important source of additional information, and it has only begun to be explored. It can provide a number of model-independent probes of early galaxies that would complement inferences made based on the angle-averaged power spectrum. In particular, the dominant μ^2 term of the anisotropy acts as a cosmic clock, its sign changing as it tracks various cosmic milestones; for instance, measuring it to be negative during reionization would directly confirm the inside-out topology of this transition (i.e. where overdense regions reionize first). Another example of a possible model-independent signature is the streaming velocity with its associated strong BAO features (Chap. 13). In addition, the global 21-cm spectrum (Sec. 15.5) is a wonderfully complementary probe of the same cosmic history. One way to express this is that the 21-cm fluctuations can be written as a product of the mean intensity and its relative fluctuations, and information on the global spectrum helps to separate these two quantities and thus break a degeneracy. It is also possible that the global 21-cm experiments will achieve a detection of the cosmic 21-cm signal before the interferometers, in which case it will be the global signal which yields the first observational estimates of when the early cosmic milestones occurred.

In part II of this volume we have focused much of the discussion on the 21-cm power spectrum (including its angular anisotropy). There are good reasons for this, even though it is not an open and shut case as in CMB studies, where the

power spectrum carries the most important cosmological information in the signal (which is thought to reflect the underlying Gaussian random field of primordial perturbations). In general, there are two different modes for studying galaxies: The collective (galaxy clustering) and the individual (studying individual galaxies). Studies of 21-cm cosmology during cosmic dawn and the EOR will be dominated by the collective regime. The 21-cm fluctuations will be dominated by various radiation fields, and the intensity of those fields at any point will be made up of the contributions of many individual sources, except perhaps in a few rare regions. The structures that will be seen will be a collective effect, and thus mainly dependent on the clustering of sources. The power spectrum naturally measures this clustering. More specifically, the distribution of sources throughout this era is driven by the underlying density distribution of matter (except for the additional effect of the streaming velocity). This density distribution is determined by the power spectrum, and for linear fluctuations, the 21-cm map is also determined by its power spectrum (which is the underlying power spectrum times a window function, corresponding to a convolution in real space that accounts for the spatial redistribution of photons of the various relevant frequency regimes). It is true that there are some non-linear distortions along the way, but still, on the (relatively large) scales resolvable by upcoming radio arrays, the power spectrum should capture most of the information available in a full image. Indeed, as described throughout this part, the 21-cm power spectrum can be used to reconstruct the most interesting astrophysical information that we desire: at what redshifts $\text{Ly}\alpha$ coupling, cosmic heating, and reionization occurred, how fast they progressed, which galactic halos dominated each era, and what the spectrum was of the sources (e.g. the X-ray spectrum in the case of X-ray heating). The most non-linear process is reionization (with its sharp edges in the expected scenario in which it is dominated by UV photons), but the non-Gaussianity of the ionization field only reflects the rapid absorption of ionizing photons, and may not probe much interesting physics beyond that. Also, in the near future the power spectrum is likely to be the main available observable from the least explored, and thus most exciting, high-redshift regime of the pre-EOR cosmic dawn; imaging from such an early time will be quite difficult even for the SKA.

That said, the non-Gaussianity of 21-cm fluctuations [5] does make other statistics beyond the power spectrum interesting, including the bispectrum [6, 7], the 21-cm PDF (probability distribution function, i.e. histogram of values of the 21-cm brightness temperature) [8–13], and the difference PDF (i.e. histogram of T_b differences between pixel pairs) [14, 15]; some of the additional information available in the PDF can be captured by its skewness [16, 17].

While in this work we have focused heavily on the emerging field of 21-cm cosmology, other cosmological probes are making rapid advances and should explore some complementary aspects of high-redshift galaxies. The James Webb Space Telescope (JWST; <http://www.jwst.nasa.gov/>) should discover at least the largest galaxies at early times, as well as rare bright objects (such as

supernovae or gamma-ray bursts) in more typical galaxies. The planned generation of larger ground-based optical/IR telescopes, including the Thirty Meter Telescope (TMT; <http://www.tmt.org/>), the Giant Magellan Telescope (GMT; <http://www.gmto.org/>), and the European Extremely Large Telescope (E-ELT; <http://www.eso.org/public/teles-instr/e-elt/>) should give us detailed, spectroscopic information on some of these objects and their surrounding IGM. Imaging the 21-cm sky, as planned for the SKA, will be very interesting around particular bright objects. In another area, the CMB, in addition to its further development as a cosmological probe, may allow the detection of the small-scale signature of CMB scattering by the ionized bubbles during cosmic reionization [18–21].

We have also discussed in this work the complementary interaction in this field between numerical simulations, analytical (or semi-analytical) models, and semi-numerical methods. Each method has its advantages and disadvantages, and in particular it is important not to overlook the limitations of numerical simulations (Sec. 11.3).

Another highlight of this work is in pointing out how the idea of unusually large fluctuations in the number density of high-redshift galaxies (Sec. 11.2) is a common thread that has driven the whole topic of 21-cm fluctuations, from the understanding of the character of reionization (Sec. 14.1) to the first predictions of large-scale 21-cm fluctuations from the inhomogeneous Ly α (Sec. 15.2) and X-ray (Sec. 15.3) backgrounds. It has recently been joined by an exciting new source of large-scale fluctuations, the supersonic streaming velocity (Chap. 13). This new source comes with a strong signature of baryon acoustic oscillations, making it a potential tool for identifying the presence of tiny, million solar mass halos at very early times. The streaming velocity certainly had a major effect on the first generation of stars, and it may also have been significant at redshifts that are observable with 21-cm experiments (Sec. 15.3), though this depends on just how efficiently such small halos were able to form stars. Within the subject of basic 21-cm physics, we have also highlighted the low-temperature corrections to the basic expressions of 21-cm cosmology (Sec. 12.2).

In this work we have focused on the astrophysical era of 21-cm cosmology that is accessible to upcoming experiments. However, it is also important to keep in mind the great long-term promise of the development of 21-cm cosmology. When 21-cm measurements reach small spatial scales, this will open up a variety of new probes and applications, especially in the dark ages during which 21-cm cosmology will be a clean cosmological probe. For example, 21-cm fluctuations should be present down to much smaller scales than CMB fluctuations (which are cut off by the combination of Silk damping and the width of the surface of last scattering; see Sec. 4.8.2). This implies a far greater potential sensitivity of 21-cm measurements to a small primordial non-Gaussianity [22, 23]. Measuring the primordial power spectrum on small scales will also probe the tilt of the power spectrum and could potentially uncover a cutoff due to dark matter properties (such as in the warm dark matter

or fuzzy dark matter [24] models). Also, the gas temperature can in principle be mapped through its effect on the small-scale power spectrum (i.e. the filtering mass discussed in Sec. 11.1.2) as well as more directly through the anisotropic effect of the thermal smoothing of the 21-cm power spectrum [25]; e.g. if the cosmic gas is radiatively heated to 10^3 K, then the smoothing is expected on a scale of ~ 20 kpc. On small scales, the supersonic streaming velocity also has a significant effect on the 21-cm power spectrum [26]. Further back in time, a 21-cm signal is expected from the cosmological epoch of recombination [27].

We would like to end this work in the same way that the author concluded a review written more than a decade ago [28], with the sincere hope of not having to write this again in the future: Astronomers are eager to start tuning into the cosmic radio channels of 21-cm cosmology.

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Kentaro Nagamine

*Osaka University
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Preface

Cosmology is a field of study that deals with everything within our Universe and beyond. It is a rich field that involves many scientific disciplines such as physics, astronomy, chemistry, biology, and many more. Strong and sound interaction between theory and observations is another unique feature of this field. Thanks to observational and theoretical studies over the past few decades, we now have a standard concordance cosmological model that is dominated by dark energy and dark matter, the so-called Λ cold dark matter (Λ CDM) model.

In cosmology, we need to deal with vast scales in cosmos from Gpc down to AU, which prohibits us to perform realistic experiments in our laboratory. However, using physical theories and scientific imagination, we can perform realistic experiments of structure formation in our Universe using supercomputers. This is the field of *Numerical Cosmology* (or *Computational Cosmology*), which made tremendous advancement since 1980s along with the improvement of supercomputers.

As I became a university faculty and started to teach graduate students in my *Cosmology* class, I realized that there are no good, updated textbooks on numerical cosmology. This field progresses so rapidly day by day that anyone who keeps track of the frontier would hesitate to write a textbook on this subject; there is a fair chance that some parts of it will become obsolete by the time one finishes writing it.

The approach that this new textbook series has attempted to take is to update the series more frequently than the traditional textbooks and catch up with the advancements in the field as quickly as possible, utilizing the online technological development as much as possible. For this particular volume on *Numerical Cosmology*, we have also taken the omnibus approach, in which multiple authors write individual chapters of their choice, allowing them to focus on the details of each subject. The drawback of this method is a possible lack of consistency throughout the volume and some overlaps between chapters. However, we have left some of these overlaps intentionally without controlling each author, because the students may actually benefit from the different ways of explaining the same topic.

This textbook targets fresh graduate students who are trying to get started in this field, or anyone else who is already in the field of astronomy and astrophysics, but would like to know more about numerical cosmology. Each chapter is more or less independent of each other, therefore one can start reading from any chapter if one is already familiar with the introductory material in Chapter 1. We hope that many students and young researchers will find this textbook useful and consider joining the exciting endeavor in numerical cosmology.

This volume has a natural and obvious flow in its organization. We start with a brief overview of cosmological studies in Chapter 1 with some history of numerical cosmology. In Chapters 2 and 3, we review the methodology of cosmological N -body and hydrodynamic simulations. From Chapter 4 onwards, we roughly follow the cosmological timeline and the structure formation in our Universe: first stars (Chapter 4), first galaxies and black holes (Chapter 5), galaxy formation (Chapter 6), secular evolution of disk galaxies (Chapter 7), evolution of cosmic gas (i.e., intergalactic medium and circumgalactic medium; Chapter 8), and the formation and evolution of galaxy clusters (Chapter 9). While this list is not complete, it covers a wide range of subjects that are studied in the field of computational cosmology today.

As the editor, I am extremely grateful to all chapter authors who took time out of their busy schedules to write each chapter and tolerated my frequent email follow-up for their files. Without their dedication to science and education, this volume would not have existed, and the full credit for this book goes to all authors of individual chapters.

I would also like to express my sincere gratitude to all of my mentors, collaborators, and colleagues who guided me throughout my research career. There are simply too many to name all of them here, but most notably, I have learned a great deal by writing papers with the following people in the early days of my career: Jerry Ostriker, Renyue Cen, Masataka Fukugita, Lars Hernquist, Volker Springel, Art Wolfe, and Mike Norman. Finally, I would like to thank my family, who have provided gracious support while I worked on putting this volume together and throughout my research career.

Kentaro Nagamine
Osaka, Japan
2017

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List of Videos

1. The idea of the hierarchical growth of structures has shaped our understanding of the formation of galaxies in the universe for many years. The movie shows, within a selfconsistent cosmological context, the formation of a disk galaxy from a redshift of $z = 10$ to $z = 0.45$, where it suffers a major merging event with another massive disk galaxy. This causes a starburst and changes the morphology of the two galaxies that then form a single spheroidal galaxy. Credit: David Schlachtberger.
<https://www.youtube.com/watch?v=Je53JQhpTfk&index=7&list=PL5xo8wI0oOBy>
2. The picture shows a visualization of Box0/mr from the Magneticum simulation set. The shown region spans a total size of 3800 Mpc. At $z = 0.0$ it contains a total number of 1.86×10^{11} dark matter, gas, star and black hole particles. Visualized is the gas which fills the space between the galaxies (color coded according to its temperature from cold/brown to hot/light blue) together with the galaxies and stars forming in the simulation (colored in white). Credit: Dolag *et al.* (2015).
<http://www.magneticum.org/media.html#Box0>
3. The movie shows a visualization of the time evolution of Box2/hr from the Magneticum Pathfinder simulation set. The view at the beginning spans a total size of 500 Mpc and then zooms onto the most massive cluster forming within the simulation. Visualized is the gas which fills the space between the galaxies (color coded according to its temperature from cold/brown to hot/light blue) together with the galaxies and stars forming in the simulation (colored in white). Credit: Klaus Dolag (USM, LMU)
https://www.youtube.com/watch?v=HHh_BcQ6fbQ&list=PL5xo8wI0oOByhvXeb-cB
4. Numerical simulation of evolution of the vertical structure in the stellar bar and its vertical buckling instability: edge-on-view along the bar minor axis. The length on the axes is given in kpc and the shades of gray represent the projected density of stars. The time in billions of years (Gyrs) is given at the top. The bucklings correspond to maximal vertical asymmetries, the first at about 2.4 Gyr and the second one between 5–8 Gyr. Note the bar flip-flops between 2.3 Gyr

and 2.4 Gyr, and develops a persistent vertical asymmetry during the second buckling. The result of the vertical buckling instability is a boxy and peanut-shaped bulge, which grows with every buckling.

<https://youtu.be/seiQ5SmGKuU?list=PLW1jtByUJvcs3EY3UlnQihnNpuStlo7gR>

5. Cosmological numerical simulations of evolution of the DM halo in the $R-v_R$ phase space (R is the spherical radius from the halo center, and v_R is the radial velocity of the dark matter and baryons). Two models are shown: the pure dark matter (PDM) halo evolution (top frame), and the dark matter with baryons (BDM) halo evolution (bottom frame). Both models have identical initial conditions and differ only by the absence/presence of baryons. Only evolution of dark matter is shown in both models. Redshift is shown in the lower right corners. The simulations are shown from $z = 25$ to $z = 0$. Note the appearance of “fingers,” representing tidal disruption of merger companions, and the appearance of the shell structure inside and outside of the main halo. The colors correspond to the dark matter particle density on the $R-v_R$ surface. The vertical arrow shows the halo virial radius, R_{vir} , the dashed white line is $v_R = 0$, and blue line is the average v_R at each R . The velocity axis is normalized by the virial velocity, v_{vir} .
https://youtu.be/BriGHLC_NDU?list=PLW1jtByUJvcs3EY3UlnQihnNpuStlo7gR
6. Formation of a galaxy cluster.
<https://youtu.be/jrufJf6AsvM?list=PLW1jtByUJvcs3EY3UlnQihnNpuStlo7gR>
7. The different internal components of galaxy clusters like galaxies, ICM, IGM and ICL and their interactions.
<https://youtu.be/zyGiVyq5FQ0?list=PLW1jtByUJvcs3EY3UlnQihnNpuStlo7gR>
8. C2PAP CosmoSim — A web portal for hydrodynamical, cosmological simulations
https://www.youtube.com/watch?v=J_8hGaPOnr0&index=1&list=PL5xo8wI0oOBy

(Below we also give some examples of code and movie websites of cosmological simulations.)

9. CosmoSim project: <https://www.cosmosim.org/>
10. EAGLE project:
<http://eagle.strw.leidenuniv.nl/index.php/eagle-visualisation/>
11. Enzo Project: <http://enzo-project.org/>
12. FIRE project (Gizmo): <http://fire.northwestern.edu/visualizations/>
13. GADGET-2: <http://wwwmpa.mpa-garching.mpg.de/gadget/>
14. Horizon-AGN project (RAMSES): <https://www.horizon-simulation.org/media.html>
15. Illustris project (AREPO): <http://www.illustris-project.org/media/>
16. Illustris-TNG project (AREPO): <http://www.tng-project.org/media/>
17. Magneticum project: <http://www.magneticum.org/media.html#MOVIES>
18. RAMSES movies: <http://www.itp.uzh.ch/~teyssier/ramses/Movies.html>

Chapter 1

Overview: Cosmological Framework and the History of Computational Cosmology

Kentaro Nagamine

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This chapter presents an overview of cosmological framework that is necessary to perform cosmological simulations. First, we start with a brief history of cosmological studies of the Universe, such as the discovery of Hubble's law and cosmic microwave background radiation which constitute the major observational evidence of expanding Big Bang cosmology. Second, we present the basics of General Relativity theory and Friedmann models that describe the expanding universe. Under this theoretical framework, we introduce various cosmological parameters and current best-fit Λ cold dark matter (CDM) model. Third, we discuss the history and development of computational cosmology which was achieved concurrently with the evolution of supercomputers.

1.1. Brief history of cosmological studies

Cosmology, which is the study of our Universe and the structures within, has advanced tremendously over the last 50 yrs. Physical and theoretical basis of cosmology was provided by the theory of General Relativity by Albert Einstein in 1915–1916 [1–5]. About a decade later, Edwin Hubble discovered in 1929 [6] that more distant galaxies were receding from us with faster speeds, i.e., the Hubble's law. A natural explanation of this observational data is given by considering a raisin bread baked in an oven, where equally spaced raisins (i.e., galaxies) become farther apart from each other as the dough expands isotropically. In this raisin bread universe, whichever raisin you live in, the same observational data can be obtained as the Hubble's law for the recession velocity of other raisins, thereby explaining both expansion and isotropy of the Universe beautifully.

Then, A. A. Penzias and R. W. Wilson discovered the cosmic microwave background (CMB) radiation in 1965 [7], and its theoretical interpretation as the remnant radiation of the Big Bang was provided by R. H. Dicke *et al.* in [8]. Today, the expanding Big Bang model is supported by the following three major observational evidences:

- (1) Hubble’s law,
- (2) CMB Radiation,
- (3) Big Bang nucleosynthesis.

The first pillar supporting the Big Bang cosmology is Hubble’s law, which states that the distant galaxies recede from us with speeds that are proportional to their distances, i.e.,

$$v = H_0 d. \quad (1.1)$$

This is also called the Hubble flow. The current Hubble parameter H_0 is usually expressed in units of $\text{km s}^{-1} \text{Mpc}^{-1}$, velocity v in units of km s^{-1} , and distance d in units of megaparsec (Mpc). Its current best estimate is about

$$H_0 \approx 70 \text{ km s}^{-1} \text{Mpc}^{-1}, \quad (1.2)$$

based on the Cepheid distance scale and the CMB temperature anisotropy [9–12]. We often use the normalized, unitless Hubble parameter

$$h \equiv \frac{H_0}{100 \text{ km s}^{-1} \text{Mpc}^{-1}} \approx 0.7. \quad (1.3)$$

The latest WMAP and Planck satellite results [11, 12] give slightly lower values than 0.7, $h \approx 0.67\text{--}0.70$. Given that H_0 has units of $[1/\text{Time}]$, its inverse gives a rough estimate of the age of the Universe,

$$t_H \approx H_0^{-1} \approx 14 \text{ Gyr}, \quad (1.4)$$

which is called the Hubble time. By coincidence, this is very close to the current best estimate of cosmic age, $t \approx 13.8 \text{ Gyr}$ by WMAP and Planck [11, 12]. Other cosmological parameters will be introduced in the next section.

The second pillar is the CMB that has a black-body spectrum of $T \approx 2.73 \text{ K}$ at the present time, as measured by the COBE satellite in 1994 [14]. It is often said that the CMB is the most perfect black-body spectrum in the Universe. The CMB temperature distribution in the sky has tiny fluctuations of the order $\Delta T/T \sim 10^{-5}$ (Fig. 1.1), and this anisotropy provides a definite physical scale that can be used as a “standard ruler”. In the early Universe, baryons and photons were tightly coupled, and they were oscillating together. This acoustic oscillation produces hot and cold spots in the CMB, and we can infer the curvature of spacetime by measuring the angular scales of this temperature anisotropy. The statistical nature of CMB

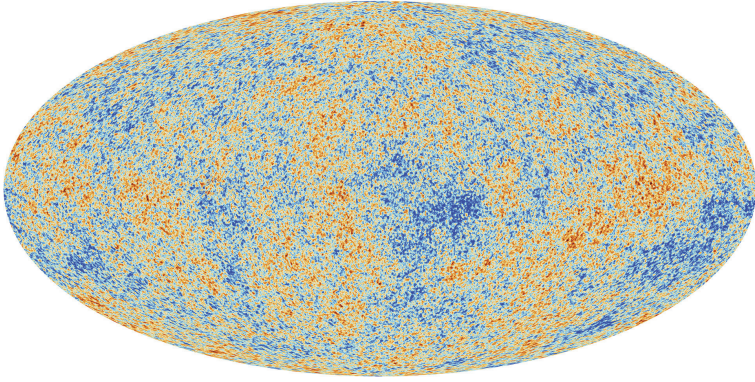


Fig. 1.1. Temperature anisotropy in the CMB radiation observed by the Planck satellite [13]. It is the baby picture of our Universe at about 380,000 yrs after the Big Bang.

Image credit: ESA and the Planck Collaboration, http://www.esa.int/spaceinimages/Images/2013/03/Planck_CMB.

anisotropy is represented by the angular power spectrum of temperature anisotropy. First, the temperature anisotropy is expanded in spherical harmonics,

$$\frac{\Delta T}{T}(\hat{\mathbf{n}}) = \sum_{\ell, m} a_{\ell}^m Y_{\ell m}(\hat{\mathbf{n}}). \quad (1.5)$$

The angular autocorrelation function $C(\theta)$, which measures the correlation of temperature anisotropy between two spots in the sky separated by an angle θ , is defined by

$$C(\theta) = \left\langle \frac{\Delta T}{T}(\hat{\mathbf{n}}_1) \frac{\Delta T}{T}(\hat{\mathbf{n}}_2) \right\rangle, \quad (1.6)$$

where $\hat{\mathbf{n}}_1 \cdot \hat{\mathbf{n}}_2 = \cos \theta$. The angular autocorrelation function can also be written as

$$C(\theta) = \frac{1}{4\pi} \sum_{\ell} \sum_{m=-\ell}^{m=+\ell} |a_{\ell}^m|^2 \mathcal{P}_{\ell}(\cos \theta) \quad (1.7)$$

$$= \frac{1}{4\pi} \sum_{\ell} (2\ell + 1) \mathcal{C}_{\ell} \mathcal{P}_{\ell}(\cos \theta), \quad (1.8)$$

where $\mathcal{P}_{\ell}$ is the Legendre polynomial function, and $\mathcal{C}_{\ell} = \langle |a_{\ell}^m|^2 \rangle$ is the expectation value of the square of the harmonic coefficients. Usually, a broadband measure of the power per log ℓ is defined as

$$\mathcal{D}_{\ell}^{TT} = \frac{\ell(\ell + 1)}{2\pi} \mathcal{C}_{\ell} \quad (1.9)$$

and plotted as in Fig. 1.2. Here, we can see the most prominent first acoustic peak at the mode of $\ell \sim \pi/\theta \approx 200$ (at ~ 1 degree), and the best-fit Λ CDM model is shown with a solid line. The data points and the Λ CDM model prediction beautifully agree

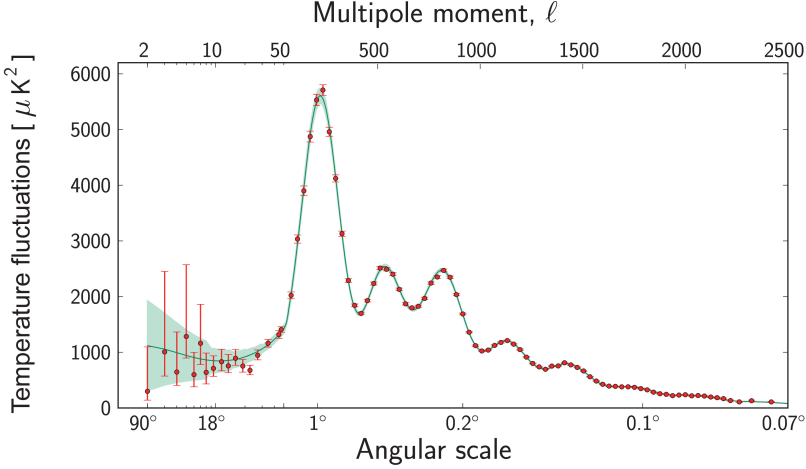


Fig. 1.2. Angular power spectrum of temperature anisotropy in the Planck CMB data [17]. Here, the scale of abscissa changes from logarithmic to linear at the “hybridization” scale, $\ell = 29$. The multipole moments and corresponding angular scales are shown at the top and bottom axes. The red dots are the Planck observational data, and the solid line is the best-fit Λ CDM model.

Image credit: ESA and the Planck Collaboration, http://www.esa.int/spaceinimages/Images/2013/03/Planck_Power_Spectrum.

with each other to higher ℓ modes, however the error bars become larger at large scales (i.e., small ℓ) due to cosmic variance. In other words, we can observe only one universe, and we run out of sampling points at very large angles. Following review articles on CMB would be useful for more reading for students [15, 16].

1.2. Cosmological framework

1.2.1. General Relativity and Friedmann–Robertson–Walker metric

In General Relativity theory, the spacetime interval of two events is written by

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu, \quad (1.10)$$

where $g_{\mu\nu}$ is the metric tensor which describes the structure of spacetime. The indices μ and ν run from 0 to 3 corresponding to (x^0, x^1, x^2, x^3) , where $x^0 = t$ is the time and the rest are spatial coordinates. In the regime of Special Relativity where the discussion is limited to the inertial frame with no acceleration, it simplifies to the Minkowski metric:

$$g_{\mu\nu} = \eta_{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 \end{pmatrix}. \quad (1.11)$$

Note that we adopt the sign convention of $(-1, +1, +1, +1)$ throughout this text-book series.

In General Relativity, spacetime is described by the Einstein equation:

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + \Lambda g_{\mu\nu} = \frac{8\pi G}{c^4}T_{\mu\nu}, \quad (1.12)$$

where $R_{\mu\nu}$ is the Ricci tensor, R is the Ricci scalar, Λ is the cosmological constant, G is the gravitational constant, c is the speed of light, and $T_{\mu\nu}$ is the energy-momentum tensor. Note that the signs of the last term of left-hand side (LHS) and the right-hand side (RHS) of Eq. (1.12) can change according to the adopted sign convention. One can find a detailed derivation of this equation in Ref. [18, Chapter 7]. Sometimes, the “Einstein tensor” is defined as $G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}$. The cosmological constant Λ was originally written as a pure constant by Einstein, however, its notion has been generalized to “Dark Energy” which could depend on both space and time. In other words, dark energy can be regarded as a “field” that resides in vacuum, which is the concept coming from quantum field theory. The Einstein equation describes how the spacetime on the LHS responds to the energy and momentum on the RHS.

Einstein argued that our Universe is isotropic and homogeneous on large scales, which is called the “Cosmological Principle”. Under this assumption, our Universe can be described well by the Robertson–Walker metric:

$$g_{\mu\nu}^{\text{RW}} = \begin{pmatrix} -c^2 & 0 & 0 & 0 \\ 0 & \frac{a^2(t)}{1 - kr^2} & 0 & 0 \\ 0 & 0 & a^2(t)r^2 & 0 \\ 0 & 0 & 0 & a^2(t)r^2 \sin^2 \theta \end{pmatrix}, \quad (1.13)$$

and the spacetime interval can be written as

$$ds^2 = g_{\mu\nu}^{\text{RW}} dx^\mu dx^\nu = -c^2 dt^2 + a^2(t) \left\{ \frac{(dr)^2}{1 - kr^2} + r^2 d\Omega \right\}, \quad (1.14)$$

where $a(t)$ is the scale factor, r is the comoving coordinate, k is the curvature, and $d\Omega \equiv (d\theta)^2 + \sin^2 \theta (d\phi)^2$. In this case, the spatial coordinates are $(x^1, x^2, x^3) = (r, \theta, \phi)$. An isotropic and homogeneous universe that can be described by Eq. (1.13) is called the “Friedmann–Robertson–Walker (FRW)” universe.

The scale factor $a(t)$ expresses the expansion of the universe, and its range is usually taken as $[0, 1]$, from the Big Bang ($a(0) = 0$) to the present time ($a_0 \equiv a(t_0) = 1$). In the field of cosmology, physical quantity at the present time is often written with a subscript zero.

Inserting Eq. (1.13) into Eq. (1.12), one obtains the so-called Friedmann equations:

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\rho - \frac{kc^2}{3} + \frac{\Lambda c^2}{3}, \quad (1.15)$$

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}\left(\rho + \frac{3p}{c^2}\right) + \frac{\Lambda c^2}{3}, \quad (1.16)$$

where ρ is the *mass* density of the Universe, and p is the pressure. Equation (1.15) is the 0-0 component of Einstein equation.

1.2.2. Cosmological parameters and Λ CDM model

The Hubble parameter $H(t)$ and the critical mass density of the Universe ρ_c are, respectively, defined by

$$H(t) \equiv \frac{\dot{a}}{a}, \quad \rho_c(t) \equiv \frac{3H^2}{8\pi G}. \quad (1.17)$$

It is useful to remember the present day value of critical mass density,

$$\rho_{c,0} \equiv \frac{3H_0^2}{8\pi G} = 1.88 \times 10^{-29} h^2 \text{ [g cm}^{-3}\text{]} \quad (1.18)$$

$$= 2.775 \times 10^{11} h^2 \text{ [M}_\odot \text{ Mpc}^{-3}\text{]}. \quad (1.19)$$

Combining Eqs. (1.15) and (1.17) yields

$$\Omega_M + \Omega_k + \Omega_\Lambda = 1, \quad (1.20)$$

where

$$\Omega_M \equiv \frac{\rho}{\rho_c}, \quad \Omega_k \equiv -\frac{kc^2}{3H^2}, \quad \Omega_\Lambda \equiv \frac{\Lambda c^2}{3H^2} \quad (1.21)$$

are the nondimensional energy density parameters of matter, curvature, and cosmological constant, respectively. More generally, one could also consider the energy densities of baryons (Ω_b), dark matter (Ω_{DM}), neutrinos (Ω_ν), or radiation (Ω_r), in which case the LHS of Eq. (1.20) will become the sum of all components under consideration. In terms of redshift $z \equiv (1/a) - 1$, the Hubble parameter can be written as

$$H(z) = H_0 \sqrt{\Omega_M(1+z)^3 + \Omega_k(1+z)^2 + \Omega_\Lambda}. \quad (1.22)$$

The current best estimates lie close to

$$(\Omega_M, \Omega_b, \Omega_k, \Omega_\Lambda, h, n_s, \sigma_8) \approx (0.3, 0.04, 0.0, 0.7, 0.7, 0.96, 0.8) \quad (1.23)$$

from a combination of various measurements, such as CMB anisotropy [11, 12], Cepheids [10], distances to Type Ia supernovae, galaxy cluster abundance, baryon acoustic oscillation, gravitational lensing, etc. All combinations of these various

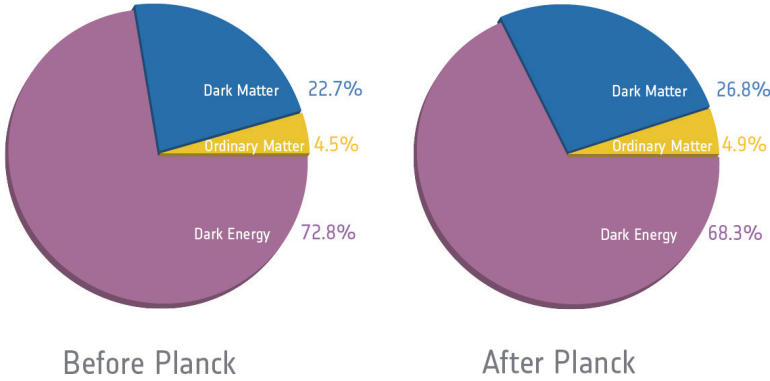


Fig. 1.3. Cosmological energy density fractions of dark energy, DM, and ordinary matter, estimated from the WMAP (left) and Planck (right) satellites. Both observations suggested a flat Universe, therefore the total energy density parameter adds up to 100%, i.e., $\Omega_{\text{tot}} = 1.0$.

Image credit: ESA and the Planck Collaboration, http://www.esa.int/spaceinimages/Images/2013/03/Planck_cosmic_recipe.

observational data point to the so-called “ Λ cold dark matter” (Λ CDM, or sometimes also written as LCDM) universe, which is dominated by dark matter (DM) and dark energy [19, 20]. Thanks to the recent advancement of observational constraints, we now know the values of these parameters with an accuracy better than 10% (Fig. 1.3).

In Eq. (1.23), we also introduced two additional parameters that we need to describe structure formation in the Universe. First is the spectral index “ n_s ” of the primordial power spectrum

$$P(k) \equiv V_u \langle |\delta_{\mathbf{k}}|^2 \rangle \propto k^{n_s}, \quad (1.24)$$

which describes the distribution of matter fluctuations in the Fourier space in the early Universe. Here, $\delta_{\mathbf{k}}$ is the Fourier transform of the overdensity field $\delta(\mathbf{x}) = (\rho(\mathbf{x}) - \bar{\rho})/\bar{\rho}$,

$$\delta_{\mathbf{k}} = \frac{1}{V_u} \int \delta(\mathbf{x}) \exp(-i\mathbf{k} \cdot \mathbf{x}) d^3\mathbf{x}, \quad (1.25)$$

and V_u is some large cosmological volume that is representative of the Universe.

Second is the variance of fluctuations “ σ_8 ” at a scale of $R = 8 \text{ Mpc}/h$, which gives the normalization of $P(k)$ at the present day. The scale of $R = 8 \text{ Mpc}/h$ is chosen because the variance in galaxy distribution is known to be close to unity at this scale. For a scale of R , variance and power spectrum are related to each other via

$$\sigma(R) \equiv \langle \delta^2(\mathbf{x}; R) \rangle = \frac{1}{(2\pi)^3} \int_0^\infty P(k) \tilde{W}_R^2(k) d^3k, \quad (1.26)$$

where $W_R(k)$ is the window function for smoothing the density field at a scale R . A well-known example of a window function is the top-hat filter

$$W_R(\mathbf{x}) = \frac{1}{V} \begin{cases} 1 & \text{for } |\mathbf{x}| < R, \\ 0 & \text{for } |\mathbf{x}| \geq R, \end{cases} \quad (1.27)$$

where $V = 4\pi R^3/3$ is the volume inside the filter, and its Fourier transform is

$$\tilde{W}_R(k) = \frac{3\{\sin(kR) - kR \cos(kR)\}}{(kR)^3}. \quad (1.28)$$

When we observe or simulate the Universe, we cannot take measurements at infinite number of points in space, therefore the measurement and comparison have to be carried out at limited sampling points of *smoothed* density field on a certain spatial scale. Above smoothing kernel W_R takes care of this smoothing process.

A statistic that is often used to describe the distribution of galaxies and matter is the two-point correlation function

$$\xi(\mathbf{r}) \equiv \langle \delta(\mathbf{x})\delta(\mathbf{x} + \mathbf{r}) \rangle, \quad (1.29)$$

which is just a Fourier transform of the power spectrum,

$$\xi(r) = \frac{1}{V_u} \sum_{\mathbf{k}} P(k) e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{(2\pi)^3} \int P(k) e^{i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r}. \quad (1.30)$$

Note that $\xi(r)$ depends only on the absolute value of distance $r = |\mathbf{r}|$ under the assumption of homogenous and isotropic universe. As we will discuss in the next section, the correlation function of galaxies has been measured and used to constrain the density fluctuations for many years.

The remarkable success of Λ CDM model is summarized well in the power spectrum of matter fluctuations shown in Fig. 1.4. Here, it can be seen that the CMB data constrains $P(k)$ from large to intermediate scales ($\gtrsim 30 \text{ Mpc } h^{-1}$), overlapping with the Sloan Digital Sky Survey (SDSS) galaxy distribution constraint. It has been pointed out that CMB anisotropy measurement alone cannot determine Ω_M precisely [22] due to a strong degeneracy with other parameters. However, its degeneracy is almost orthogonal to that of the SDSS galaxy estimate, which helps significantly in tightening the constraints on all the cosmological parameters. The cluster abundance gives the normalization of $P(k)$, and the Lyman- α ($\text{Ly}\alpha$) forest observation gives constraints at smaller scales of $1\text{--}20 \text{ Mpc } h^{-1}$. Below 1 Mpc scale, it is the nonlinear regime where galaxies themselves may affect the matter distribution via feedback by supernovae and supermassive black holes.

1.2.3. CDM crisis?

While the success of Λ CDM model on large scales is quite impressive, several possible problems have been pointed out for the CDM model at the small scales of

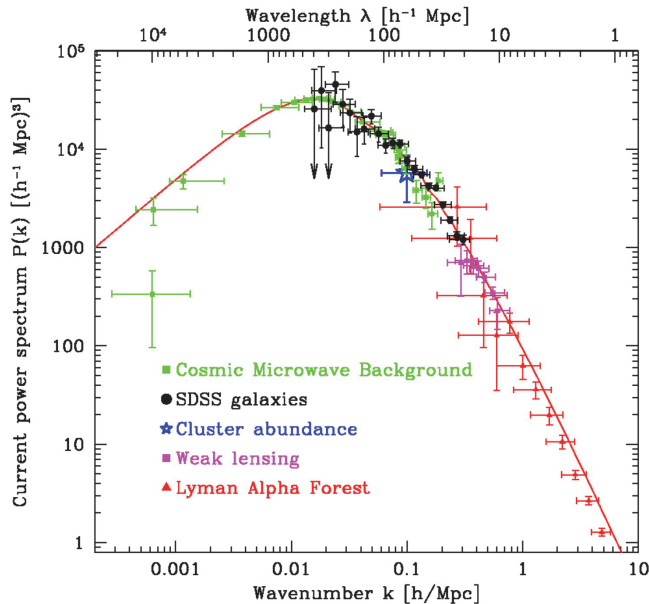


Fig. 1.4. Power spectrum of matter density field, summarizing the success of Λ CDM model on scales greater than galaxy clusters ($\gtrsim 1 h^{-1} \text{Mpc}$). Figure taken from [21].

$\lesssim 100 \text{ kpc}$ (see, e.g., [23] for a review):

- (1) core-cusp problem of DM halos,
- (2) substructure problem (or missing satellites problem),
- (3) too-big-to-fail problem [24],
- (4) galaxies in voids [25, 26],
- (5) satellite sheet distribution problem, and so on.

For example, the core-cusp problem has a long and rich history. Several early simulations [27–29] showed that DM halos have an inner density profile of $\rho \propto r^{-1}$, and the power-law slope becomes steeper to -3 (the so-called NFW profile [29]) or -4 in the outskirts. In particular, Ref. [30] argued that the NFW profile is universal in hierarchically clustering universes, irrespective of halo mass and cosmology. However, some later publications found slightly steeper inner slopes of roughly $\rho \propto r^{-1.5}$ [31–33], as well as not-so-universal profile from high-resolution N -body simulations [34, 35]. In any case, the observed dwarf galaxies that are dominated by DM seem to have flatter “cores”, apparently contradicting with steeper slopes found in N -body simulations.

However, over the years, many researchers have also pointed out repeatedly [36] that baryonic processes such as supernova (SN) feedback and active galactic nuclei (AGN) feedback may be important in changing the inner density profile of DM. For example, Refs. [37–39] showed that SN feedback can perturb the central DM

potential well, thereby flattening the DM cusp. Other possibilities are the dynamical friction on infalling gas clumps dissipating clumps' orbital energy and depositing it onto the DM [40], or bar-driven dynamics where inner Lindblad-like resonance couples the bar to the DM, transferring the bar-pattern angular momentum to the DM cusp and removes the cusp [41]. Given these various processes, the CDM model might not be contradictory with the observed DM core, once all important baryonic processes are properly taken into account.

The “substructure problem” (or the “missing satellites problem”) is about the seemingly overabundant low-mass halos in CDM simulations compared to the observed number of dwarf galaxies around the Milky Way galaxy [32, 42]. However, baryonic astrophysics might also solve this issue by simply ejecting gas by SN feedback from the shallow potential well of low-mass halos, suppressing subsequent star formation. On the observational side, more numerous ultra-faint dwarf galaxies are being discovered by deeper observations, filling the gap originally discussed between simulations and observations (e.g., [43]), and careful comparisons of high-resolution zoom-in hydrodynamic simulations with observations also suggest that accounting for the limitation of current observations can resolve the possible discrepancy between observation and theory of dwarf galaxies [44].

Alternative models such as warm dark matter (WDM) and self-interacting dark matter (SIDM) have been proposed to reconcile the seeming contradiction between CDM simulations and observed cored profile. In a WDM universe, DM particles are much lighter than CDM and the free streaming in the early Universe will erase small fluctuations, resulting in less substructure and less cuspy inner density profile. WDM model could also alleviate the missing satellites problem at the same time. However, a lower limit of $\sim 3 \text{ keV}$ for WDM particle mass has been reported from the Ly α forest analysis [45], and thermal relics with lower masses are disfavored by the data. This WDM particle mass translates to a cutoff of power spectrum at $k \gtrsim 10 \text{ Mpc}^{-1}h$ and a free-streaming mass of $\sim 2 \times 10^8 h^{-1} M_\odot$. If this estimate is correct, then it means that the WDM model alone is unable to suppress the formation of dwarf galaxies sufficiently to fully resolve the missing satellites problem. The SIDM model can make the inner density profile of DM shallower, and it could even affect the dynamics of supermassive black holes (SMBH) as it changes the galactic central density sufficiently and reduce the dynamical friction [46].

Understanding the galaxies in voids also challenges the CDM model. It is widely accepted that more massive, redder elliptical galaxies prefer higher density regions, whereas star-forming, bluer spiral and irregular galaxies prefer moderate to lower density regions, a relation known as morphology–density relation [47]. In the CDM model, this is also represented as galaxy bias [48], in the sense that more massive galaxies live in massive halos, which are more clustered than lower mass halos. However, Ref. [25] posed a problem that we still do not understand galaxy formation in voids well, and proposed to use the nearest neighbor statistic as a test. Galaxies in voids are difficult to make in cosmological hydrodynamic simulations, as they are naturally in very low-density regions, and fluctuations do not grow as fast as in

the higher density region; in particular, SPH simulations lose resolution elements at late times in voids, leading to insufficient mass resolution to deal with galaxy formation in voids. In the future, we need to keep an eye on this issue, and try to reproduce the properties of void galaxies in cosmological simulations including the nearest neighbor statistic and three-point correlation function.

At the moment, the situation seems somewhat murky; while many of the “problems” raised for the CDM might be accounted for just by baryonic effects such as SN and AGN feedback, we cannot reject the possibility of alternative models of DM such as WDM or SIDM both theoretically and observationally. A direct detection of DM particle would certainly help in making a breakthrough. It is clearly an important direction of future research in numerical cosmology.

1.3. History of computational cosmology

1.3.1. *From the first galaxy merger simulations to cosmological N -body simulations*

Once we know the initial conditions of our Universe (i.e., global cosmological parameters and random Gaussian density fluctuations), it is a natural direction of scientific research to study the structure formation as a function of cosmic time. This can be done by setting up an appropriate initial condition in a computer and running it forward in time using the laws of gravity and hydrodynamics. Let us briefly review the development of early numerical simulations in galaxy formation before we jump to the description of modern cosmological simulations.

Early attempts of astrophysical simulations of structure formation started with the study of galactic structure. The very first simulation was actually performed as a laboratory experiment by E. Holmberg in 1941 [49] without using a numerical computer. It is a famous story that he used light bulbs to represent mass elements, and gravitational forces between them were computed by measuring the light fluxes between them using photocells. Each galaxy was represented by 37 light bulbs, and he simulated a tidal encounter of two galaxies as shown in Fig. 1.5.

Many programmable numerical computers started to become available in the late 1940s, which were modeled after the IAS machine (the so-called von Neumann machine), and numerical simulations of galactic structure were performed. For example, P. O. Lindblad performed a two-dimensional numerical simulation of galactic structure using $N = 116$ bodies on the BESK computer in Sweden [50]. One can see a movie of their N -body simulation in [51].

Many important work on galaxy merger followed [52–56] as computers became faster and faster. Moore’s law states that the number of transistors in a dense integrated circuit doubles approximately every 2 yrs [57], or that the chip performance doubles every 18 months (see page 12).

Astronomers and astrophysicists gradually expanded their views to cosmological scales, and the era of cosmological simulations started in 1970s and more seriously

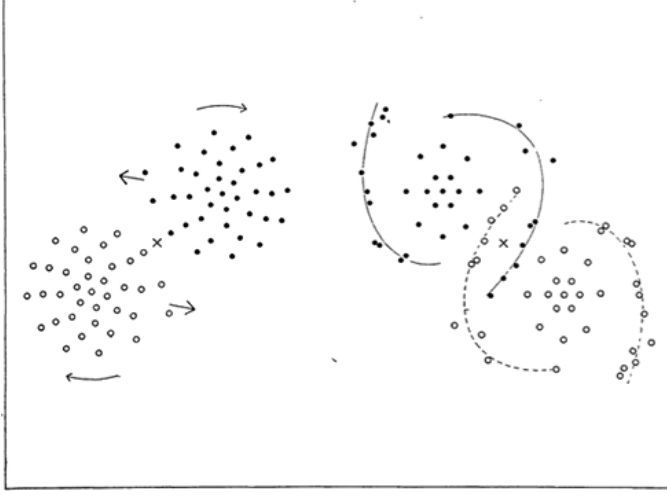


Fig. 1.5. The first N -body experiment of a galaxy encounter using 37 light bulbs for each galaxy by Holmberg. The tidal arms as a result of encounter is clearly visible on the RHS of the figure showing the final result of the experiment (or simulation). Figure adapted from Fig. 4(a) of [49].

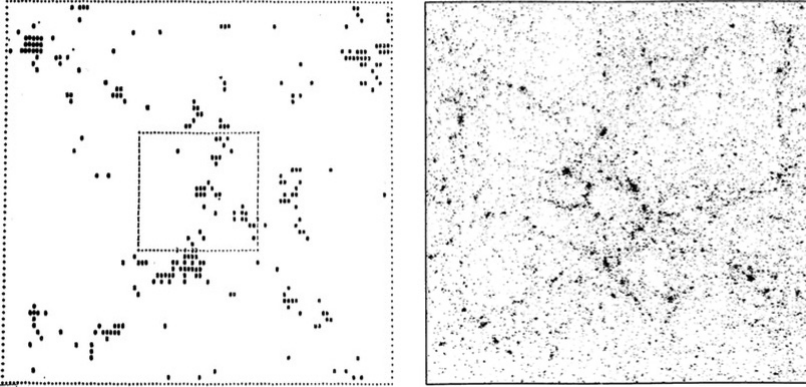


Fig. 1.6. Final snapshots of early cosmological N -body simulations by Miyoshi and Kihara [58] with $N = 400$ particles (left panel) and by Davis *et al.* [48] with $N = 32^3$ particles (right panel).

in 1980s. Perhaps, the very first cosmological N -body simulation was performed by Miyoshi and Kihara in 1975 [58] using $N = 400$ particles in an expanding universe (Fig. 1.6), with an aim of understanding the power-law behavior and time evolution of two-point correlation function $\xi(r) = (r_0/r)^\gamma$ that they had already discovered in 1969 [59] with a slope of $\gamma \approx 1.8$. Subsequent work by Peebles and Groth [60, 61] independently discovered the same features of two-point correlation function of galaxies and stimulated further work with cosmological N -body simulations. Soon

after, Aarseth *et al.* [62] performed cosmological N -body simulations with $N = 1000$ – 4000 particles in 1979.

These early simulations utilized a direct N -body summation, but soon it hits the computational time limit as it only scales as N^α ($\alpha \gtrsim 2$), and is limited to $N \lesssim 10^4$. Alternative methods such as the particle–mesh (PM; [63, 64]) and particle–particle–particle–mesh (P³M; [65–67]) were developed and achieved a better scaling of $N \log N$, which allowed them to go beyond 10^6 particles. A hierarchical tree code [68–71] has similar properties, which was later combined with the PM method, and the TreePM method [72–74] was devised in the 1990s. See Chapter 2 for further details.

Influential works in early cosmological N -body simulations in the early 1980 [48, 63] used $32^3 = 32768$ collisionless particles, reaching $N > 10^4$ particles with PM and P³M method. They were able to show a direct link between N -body simulations and observed galaxy distribution with a notion of galaxy “bias”. Today, simulations with more than several billion particles are performed. A notable example of a large N -body simulation is the Millennium simulation [75] performed by the GADGET code [76, 77] utilizing a TreePM method and $(2160)^3$ particles. The impressive structures of DM density field on various scales from the Millennium simulation are shown in Fig. 1.7.

It is interesting to observe how the largest simulations have evolved over the last two decades. Figure 1.8 shows how the simulation sizes have evolved over the years using some examples of the largest simulations performed in the field of computational cosmology. The abscissa of Fig. 1.8 shows the inverse of particle mass, m_p^{-1} , as an indicator of mass resolution, with higher values representing higher resolution. For example, the mass of a DM particle “ m_{DM} ” can be computed by

$$m_{\text{DM}} = \Omega_{\text{DM}} \rho_{c,0} L_{\text{box}}^3 / N_p, \quad (1.31)$$

where L_{box} is the comoving box size, and N_p is the total number of DM particles in the simulation. One can see that there is an anticorrelation between mass resolution and simulation volume size in Fig. 1.8, as is obvious from Eq. (1.31). The number of particles N_p that can be used for a simulation is limited by the available computational resource (i.e., amount of memory per core, the speed of each core, and how well the code is parallelized and handles the load balancing across many nodes), therefore a larger box size generally leads to higher particle masses (i.e., lower mass resolution). The details of N -body simulations and computational methods will be further described in Chapter 2, and see also Fig. 3.1.

1.3.2. Cosmological hydrodynamic simulations

Combining N -body methods with a hydrodynamical calculation has an obvious advantage of enabling more direct computations of galaxy formation and intergalactic medium (IGM), together with the evolution of large-scale structure of the Universe.

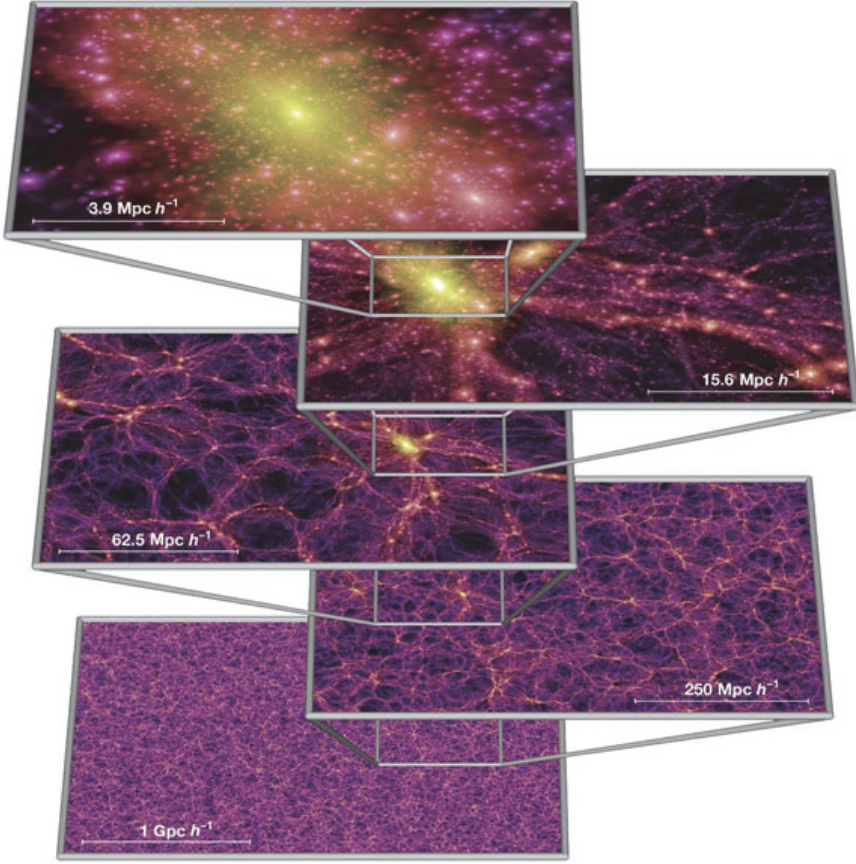


Fig. 1.7. Distribution of DM in the Millennium simulation [75], highlighting the hierarchy of large-scale structure in the Universe on different scales from a few $\text{Mpc } h^{-1}$ to $1 \text{ Gpc } h^{-1}$. In the top panel, a significant density peak is shown, which represents a galaxy cluster with many clustered DM halos. The bright spots in the picture represent significant concentrations of DM particles, i.e., DM halos. In the bottom panel, Einstein’s “Cosmological Principle” becomes apparent on scales of $>1 \text{ Gpc}$, where the large-scale structure of the universe becomes *homogeneous* and *isotropic*.

Theoretically, two major descriptions exist in fluid dynamics, i.e., *Eulerian* and *Lagrangian* methods. Eulerian method utilizes a grid [79, 80], and the fluid is described by various physical quantities in each cell, such as density, internal energy (or temperature), and pressure. Smoothed particle hydrodynamics (SPH) [81–85] is a Lagrangian method and represents fluid with gas particles, each of which is like a cloud of gas with a distribution represented by a smoothing kernel. In SPH, the density at a specific point in space can be computed by summing up the contributions from neighboring SPH particles using a smoothing kernel. Methods between Eulerian and Lagrangian are the Adaptive Mesh Refinement (AMR, see, e.g., [86]) and Moving Mesh, and a variety of codes exist for cosmological structure formation: ENZO [87], FLASH [88], ART [89, 90], and RAMSES [91] for AMR, and AREPO

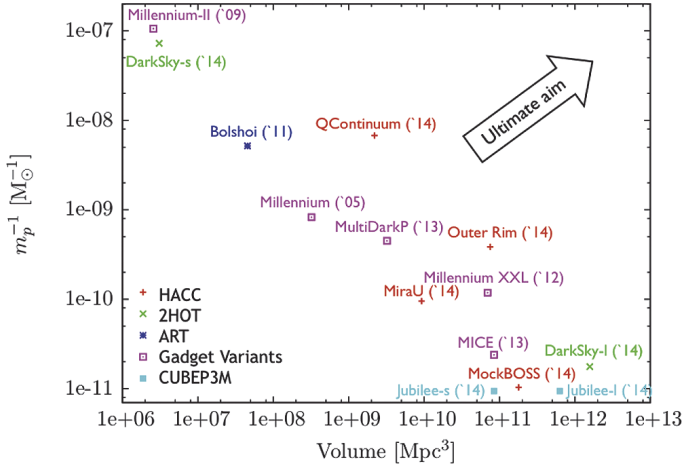


Fig. 1.8. Mass resolution vs. simulation volume for large N -body simulations. The ordinate shows the inverse of N -body particle mass, and the abscissa shows simulation volume. A higher-resolution simulation but with a smaller volume is located in the upper left of this diagram, and a lower-resolution simulation but with a larger volume is located in the right-bottom corner. The ultimate goal is to perform simulations in the upper-right corner of this diagram, but one can see that most simulations are on the diagonal line which connects above two regions. Figure taken from Fig. 1 of [78].

[92–94] for moving mesh (see also [95]). These hydrodynamic methods in cosmology will be reviewed in more detail in Chapter 3, and the details of galaxy formation modeling will be discussed in Chapter 6. Below, we briefly review the history of cosmological hydrodynamic simulations (CHS) and some milestones along the way.

A series of pioneering work in the early 1990s [96–99] studied various aspects of galaxy bias and IGM distribution successfully using an Eulerian total variation diminishing (TVD) hydrodynamic code [100] (see also [101–104]). Parallel to the Eulerian simulations, SPH method has also been used actively for galaxy formation and cosmological simulations [71, 105–109]. A public code GADGET and GADGET-2 (see [76, 77], <http://wwwmpa.mpa-garching.mpg.de/gadget/>) have been used widely for a variety of studies of galaxy formation and evolution, and its successor GADGET-3 has evolved into another public code GIZMO (see [110, 111], <http://www.tapir.caltech.edu/~phopkins/Site/GIZMO.html>).

Different codes (Eulerian, SPH, AMR, moving mesh) have their own pros and cons, and need to be investigated carefully to understand their systematic effects. Many code comparison projects have been performed, such as the Santa Barbara cluster comparison [112], Aquila project [113], and AGORA project [114] (<https://sites.google.com/site/santacruzcomparisonproject/>). Each project had its own specific goals, e.g., testing the dependence of results on N -body computational methods [115], hydrodynamic methods [112, 115, 116], or star formation and feedback models [113, 114]. For example, Ref. [112] addressed the issue of entropy core in the center of galaxy clusters and how different hydrodynamic codes exhibited

different sizes of entropy core, which has to do with the efficiency of mixing in each code (see Chapters 3 and 9 for more details on this topic).

O’Shea *et al.* [115] showed that grid-based codes such as TVD and AMR require twice the larger initial mesh number compared to the particle number of tree codes (such as GADGET N-body/SPH code) in order to achieve a comparable DM halo mass function at the low-mass end (i.e., 256^3 root grid run will be required to produce a similar DM halo mass function for a 128^3 particle tree-code run because the force resolution is basically two cells for a grid code). In this sense, a TreePM-SPH code is more efficient in solving galaxy formation in a large cosmological volume concurrently for a large sample of galaxies, however TVD or AMR codes can solve lower density IGM better for Ly α forest statistics because the baryonic resolution element does not cluster into high-density regions and stay in the intergalactic space.

Another point is that AMR codes such as ENZO can achieve a much higher dynamic range compared to SPH codes, and therefore AMR codes are more suited to resolve the collapse of single object much deeper rather than dealing with many objects at the same time. Agertz *et al.* [116] have shown that SPH codes suffer from surface tensions and unable to resolve instabilities (e.g., Rayleigh–Taylor and Kelvin–Helmoltz instabilities), and therefore more gas clumps (e.g., molecular clouds) tend to survive without being destroyed. Improved SPH formulations and new time-stepping schemes have been proposed since these problems have been pointed out [117–119], which seem to alleviate these problems compared to “classic” SPH formulations. But these code comparisons are very difficult as it is not easy to disentangle the impact of each physical model. See Chapter 3 for more details on hydrodynamic code comparisons.

A very rough sketch on the development of CHS is shown in Fig. 1.9. In the first decade of 1990s, the simulations focused on the rough link between N -body particles and galaxy distribution, correlation function, and the overall distribution of IGM. During this first decade, the spatial resolution was on the order of comoving ~ 100 kpc, and it was not possible to resolve formation of galaxies in detail, except for the sites of most massive ones. But the notion of galaxy bias relative to underlying matter distribution was already well established in the early stage [48, 96], and the link between IGM and Ly α forest was also successfully made, as well as overall census of baryons in the Universe [122–124].

In the second decade of ~ 2000 –2010, particle numbers increased dramatically together with the fast development of large-scale supercomputers. The top right panel of Fig. 1.9 shows an example of an SPH simulation by Ref. [120] using 2×216^3 particles for DM and gas. In the same paper, CHS with particle numbers up to 2×324^3 were presented for various box sizes and resolution, with a typical spatial resolution of several comoving kpc.

In the third decade of 2010s, from the need for a higher resolution to resolve galaxy formation on sub-kpc scale, zoom-in techniques have become more popular, thanks to the help from software such as the MUSIC initial condition generator [121].

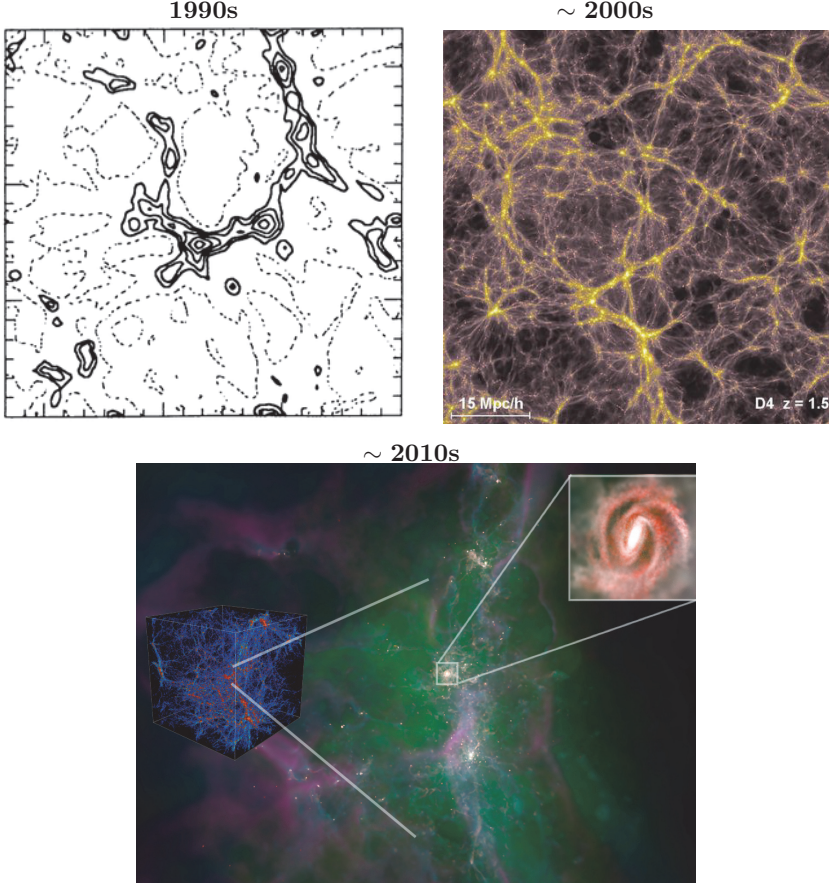


Fig. 1.9. A rough sketch on the development of CHS. Top left: One of the first large-scale CHS presented in 1990 by [104] with a box size of comoving 30 Mpc/h and 100^3 cells. Top right: A medium-sized CHS with a box size of comoving 33.75 Mpc/h and 2×216^3 particles, presented in 2003 by [120]. Bottom: A figure by Thompson and Nagamine (2014), exemplifying the zoom-in CHS technique, which has become more popular after 2010, thanks to software such as MUSIC initial condition generator [121].

In this method, one first performs a coarse N -body cosmological simulation on a large scale, say comoving $20\text{--}100\text{ Mpc } h^{-1}$. Then a DM halo of interest is identified, in which we would like to simulate galaxy formation in detail. The DM particles which formed the halo is traced back to the initial condition, and their initial positions specify the zoom-in region (typically comoving a few Mpc). We then prepare a new initial condition with a multi-level refinement with the high-resolution region populated by higher resolution gas particles (for SPH) or finer refined meshes. This method allows one to have much higher effective resolution (e.g., $1024^3\text{--}4094^3$) in the zoom-in region, while the outer low-resolution region remains at $128^3\text{--}256^3$ resolution. The drawback of the zoom-in technique is that we cannot get a large

sample of galaxies with uniform resolution in a large cosmological volume, and one cannot discuss global statistics such as galaxy luminosity function or global stellar mass density.

1.4. Summary

In this chapter, we presented an overview of background theory and current status of numerical cosmology. As discussed in Section 1.1, the progress in cosmology has been truly amazing since the 1990s, and the numerical cosmology has helped shape our view of the Universe since 1980s. As the speed of supercomputers evolve, the numerical modeling of structure formation will become more sophisticated at the same time. The spatial resolution of CHS has evolved from comoving few 100 kpc to sub-kpc scales (using the zoom-in technique) in the present day. As we approach $\lesssim 10$ pc scales, more detailed physics of ISM and star formation will be required on the smaller scales, and it will continue to be a challenge to treat and connect the large and small scales simultaneously.

We hope that this chapter has provided some glimpses of the history and current status of numerical cosmology field. In the following chapters, we will view more detailed descriptions of N -body simulations (Chapter 2), hydrodynamic methods (Chapter 3), formation of the first star (Chapter 4), galaxy formation (Chapters 5–7), cosmic gas and intergalactic medium (Chapter 8), and finally, galaxy clusters (Chapter 9).

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Chapter 2

Cosmological N -Body Simulations

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Cosmological N -body simulations play an important role in modern cosmology by providing vital information regarding the evolution of the dark matter: its clustering and motion, and properties of dark matter halos. The simulations are instrumental for the transition of the theoretical cosmology from an inspiring but speculative part of astronomy to the modern precision cosmology. In spite of more than 50 yrs of development, N -body methods are still a thriving field with the invention of more powerful methods providing more accurate theoretical predictions. Here, we review different numerical methods (PM, Tree, AMR) and ideas used in this field.

2.1. Introduction

Dark matter is an important component of the Universe. All observational evidence indicates that it dominates dynamics of normal and dwarf galaxies, clusters and groups of galaxies. At high redshifts, it provided the force that drove the formation of first galaxies and quasars. The observed large filaments and giant voids all can be understood and explained if we combine the dynamics of the dark matter with the predictions of the inflation model on the spectrum of primordial fluctuations.

The dark matter is likely made of particles that other than the gravity force do not couple with the other matter (e.g., normal gas, which for some reason in cosmology is called “baryons”. Leptons, do not take offense — you do not weigh much here). There may be some channel of interactions between dark matter particles resulting in annihilation and production of normal particles. However, even if present (no observational evidence so far), this channel is weak and the dark matter is (mostly) preserved over the evolution of the Universe.

How this dark matter evolves and how it forms different structures and objects constituted an active field of research for a very long time. The first (somewhat)

realistic N -body simulation — collapse of a cloud of 300 self-interacting particles — was carried out by P.J.E. Peebles [1]. Remember that at the dawn of cosmology, there was no dark matter, the hot X-ray gas in clusters had not yet been discovered (it was discovered in 1971), there were no voids or superclusters. So, the first N -body simulation had indicated that the force of gravity alone may be responsible for the formation of clusters of galaxies, which was a big step forward. It also discovered a problem — the density profile in the model was not right: it was too steep. The solution for this problem was continuous mass accretion on the forming cluster instead of a one-time event of collapse [2].

With the development of computer hardware and new numerical algorithms, N -body simulations became more realistic. Klypin and Shandarin [3] carried out the first 3D Particle–Mesh (PM) simulation with 32,768 particles and realistic initial conditions (nearly the same technique as used at present). The model demonstrated that the large-scale structure of the Universe should be a net of clusters of galaxies connected with filaments. The model even got a name “the chicken Universe” from one of the plots in the paper, which looked like a chicken. Davies *et al.* [4] used Particle–Particle–Particle–Mesh (P^3M) code developed by Hockney and Eastwood to run 32^3 particles with high (at that time) resolution to show that galaxies (“light”) should not follow the dark matter (“mass”). This was a very important idea. In their own words, “... kind of bias to be expected if bright galaxies form only at relatively high peaks of the linear density distribution.”

From this moment, the simulations took off. Larger and larger numbers of particles were used as new codes and new computers became available. For some time, it looked almost like a sport: whose simulation has more “muscle”. The pace has slowed down in recent years mostly because it became more difficult to analyze the simulations and to make the results accessible to the larger community.

Development of numerical methods was crucial for advances in N -body simulations. At the beginning, direct summation technique was used to run the simulations [1, 5, 6]. At that time — slower processors, no parallel computing — it was difficult to make simulations with more than just a few thousand particles. The main motivation at that time was to develop new computational methods. The number of operations in the direct summation method scales as $\propto N^2$, where N is the number of particles. So, one quickly ran out of available CPU. However, now the situation is different: processors are much faster and the number of cores on a workstation can be significant. A simulation with $N = 10^5 - 10^6$ is relatively fast (from few hours to few days). Such simulations can be very useful for testing different ideas and for small runs. It is also very easy to modify the code because everything is very transparent. For example, one can add external tidal force or modify the law of gravity. It is also a great tool for training students: a simple parallel pairwise summation code can be written in a few hours.

PM method [3, 7, 8] was a big step forward with CPU scaling $\propto N$. However, it requires a large 3D mesh for computation of the gravitational potential. The size of

a cell in this mesh defines the force resolution, and, if one needs better resolution, the number of cells should be increased. As the result, one may run out of available computer memory. Still, the PM method is very fast and is easy to implement. It is a part of all more sophisticated and faster codes.

Hybrid codes P³M [7, 9] and adaptive P³M [10] were popular for some time, but they were superseded by either adaptive mesh refinement (AMR) codes [11–14] or by Tree codes [15–19]. Older review of N -body methods can be found in [20].

2.2. Cosmological N -body problem: Main equations

In order to derive equations for the cosmological N -body problem, one can start with the equations of general relativity and derive equations of motion of self-gravitating nonrelativistic particles in the expanding Universe. For the case of nonrelativistic matter and the weak-field limit, we simply arrive at the Newtonian equations. There are some limitations with this approach: we cannot treat relativistic particles and we neglect the time needed for gravitational perturbations to travel from one point to another, effectively treating changes in the gravitational potential as instantaneous. However, these effects are not significant for most applications: velocities are typically well below that of relativistic particles and effects of the finite time of gravitational perturbations are small.

We start with definitions. Proper $\mathbf{r}$ and comoving coordinates $\mathbf{x}$ are related:

$$\mathbf{r}(\mathbf{x}, t) = a(t)\mathbf{x}(t), \quad (2.1)$$

where $a(t)$ is the expansion factor. Differentiating Eq. (2.1) over time, we get velocities:

$$\mathbf{v}(\mathbf{x}, t) \equiv \dot{\mathbf{r}} = a\dot{\mathbf{x}} + \dot{a}\mathbf{x} = H\mathbf{r} + \mathbf{v}_{\text{pec}}. \quad (2.2)$$

Here, $\mathbf{v}_{\text{pec}} = a\dot{\mathbf{x}}$ is the peculiar velocity and $H = \dot{a}/a$ is the Hubble constant. It is also useful to introduce the specific momentum defined as $\mathbf{p} \equiv a^2\dot{\mathbf{x}} = a\mathbf{v}_{\text{pec}}$.

In cosmology, we deal with a rather specific case of the N -body problem. Here, discreteness of matter can be neglected. In general, this is not the case with the two-body effects gradually accumulating over time. Systems studied in cosmology such as the nonlinear evolution of dark matter clustering do not suffer from the two-body scattering and can be treated using the collisionless Boltzmann equation paired with the Poisson equation for the gravitational potential. In the comoving coordinates, the Boltzmann equation describing the evolution of the distribution function $f(\mathbf{x}, \mathbf{p}, t)$ can be written as

$$\frac{\partial f}{\partial t} + \mathbf{x} \frac{\partial f}{\partial \mathbf{x}} - \nabla \phi \frac{\partial f}{\partial \mathbf{p}} = 0, \quad (2.3)$$

where peculiar gravitational potential $\phi(\mathbf{x})$ is related to the normal gravitational potential Φ as $\Phi = 2\pi G\rho_b r^2/3 + \phi$ where the first term is the potential of the

background (constant over space) density field ρ_b and the second term is the deviation from the background. Changing coordinates from proper $\mathbf{r}$ to comoving $\mathbf{x}$, we can write the Poisson equation as

$$\nabla^2 \phi = 4\pi G a^2 (\rho(\mathbf{x}) - \rho_b) = 4\pi G \frac{\Omega_0 \rho_{\text{cr},0}}{a} \delta_{\text{dm}}(\mathbf{x}, \mathbf{t}). \quad (2.4)$$

Here, $\delta_{\text{dm}} \equiv (\rho_{\text{dm}}(\mathbf{x}, \mathbf{t}) - \langle \rho_{\text{dm}} \rangle) / \langle \rho_{\text{dm}} \rangle$ is the dark matter density contrast. Factors Ω_0 and $\rho_{\text{cr},0}$ are the average matter (dark matter plus baryons) density in the units of the critical density and the critical density all taken at the present moment $a = 1$.

Note that the right-hand side (RHS) of Eq. (2.4) may have a positive or *negative* sign. This is unusual considering that in a normal Poisson equation, the density is always positive. The negative sign of the density term in Eq. (2.4) happens in locations where the density is below the average density of the Universe. While there are no real negative densities in the Poisson equation, the regions with the negative RHS of Eq. (2.4) in comoving coordinates act as if there are. For example, in these regions, the peculiar gravitational acceleration points away from the center of an underdense region, resulting in matter being pushed away from the center. This explains why over time voids (large underdense regions) observed in the large-scale distribution of the dark matter become bigger and more spherical.

The collisionless Boltzmann equation (2.3) is a linear first-order partial differential equation in the seven-dimensional space $(\mathbf{x}, \mathbf{p}, \mathbf{t})$. It has a formal solution in the form of characteristics: a set of curves that cover the whole space. The characteristics do not intersect and do not touch each other. Along each characteristic, the value of the distribution function is preserved. In other words, if at some initial moment t_i , we have coordinate $\mathbf{x}_i$, momentum $\mathbf{p}_i$, and phase-space density f_i , then at any later moment t , along the characteristic, we have $f(\mathbf{x}, \mathbf{p}, \mathbf{t}) = f_i(\mathbf{x}_i, \mathbf{p}_i, \mathbf{t}_i)$. Equations of the characteristics, the Poisson equation, and the Friedmann equation can be written as follows:

$$\frac{d\mathbf{x}}{da} = \frac{\mathbf{p}}{a^3 H}, \quad \frac{d\mathbf{p}}{da} = -\frac{\nabla \phi}{aH}, \quad (2.5)$$

$$\nabla^2 \phi = \frac{3}{2} \frac{H_0^2 \Omega_0 \delta_{\text{dm}}}{a}, \quad (2.6)$$

$$H^2 = H_0^2 \left(\frac{\Omega_0}{a^3} + \Omega_{\Lambda,0} \right), \quad \Omega_0 + \Omega_{\Lambda,0} = 1. \quad (2.7)$$

Here, we specifically assumed a flat cosmological model with the cosmological constant characterized by the density parameter $\Omega_{\Lambda,0}$ at redshift $z = 0$.

There are numerical factors in Eqs. (2.5) and (2.6) that obscure the fact that the equations of characteristics are nothing but the equations of motion of particles under the force of gravity. These equations are almost the equations of the N -body problem in the comoving coordinates. However, there are differences. Characteristics cover the whole phase space which we cannot do in simulations that use a finite

number of particles. Instead, we approximate the phase space by placing particles at some positions and giving them initial momenta.

How exactly we place the particles depends on the problem to be solved. For example, if a large simulation volume is expected to be resolved everywhere with the same accuracy, then particles should be nearly homogeneously distributed initially and have the same mass. If instead a small region should be resolved with a higher resolution than its environment, then we place lots of small particles in the region and cover the rest of the volume with few large particles.

Because we intend to produce an approximate solution for the continuous distribution of matter in space as described by the Boltzmann–Poisson equations, we may not even think that we solve the N -body problem — an ensemble of point masses moving under the force of gravity. For example, at the initial moment, the volume of a simulation may be covered by many small nonoverlapping cubes (not points). Then each cube is treated as a massive particle with some size, mass, and momentum. So, instead of N point masses, we have N small cubes. This is definitely a better approximation for the reality. Indeed, these types of approximations are used in many simulations. For example, in PM simulations, dark matter particles are small cubes with constant density and size. In AMR codes, particles are also cubes with the size of the cube decreasing in regions with better force resolution.

The last clarification is related to the baryons. In order to treat the baryons properly, we need to include equations of hydrodynamics and add gas density to the Poisson equation. We clearly do not do it in N -body simulations. Still, we cannot ignore baryons. They constitute a significant fraction of mass in the Universe. If we neglect baryons, there will be numerous defects. For example, the growth rate of fluctuations even on large scales will be wrong and virial masses will not be correct. In cosmological N -body simulations, we assume that all the mass — dark matter and baryons — is in particles and each particle represents both dark matter and baryons with the ratio of the two being equal to the cosmological average ratio.

2.3. Simple N -body problem: Pairwise summation

We start the discussion of numerical techniques with a very simple case: forces are estimated by summing up all contributions from all particles and with every particle moving with the same time step. The computational cost is dominated by the force calculations that scale as N^2 , where N is the number of particles in the simulation. Because of the steep scaling, the computational cost of a simulation starts to be prohibitively too large for $N \gtrsim 10^6$. However, simulations with a few hundred thousand particles are fast, and there are numerous interesting cases that can be addressed with $N < 10^6$ particles. Examples include major mergers of dark matter halos, collisions of two elliptical galaxies, and tidal stripping and destruction of a dwarf spheroidal satellite galaxy moving in the potential of the Milky Way galaxy. In these cases, it is convenient to use proper, not comoving coordinates.

The problem that we try to solve numerically is the following. For given coordinates $\mathbf{r}_{\text{init}}$ and velocities $\mathbf{v}_{\text{init}}$ of N massive particles at moment $t = t_{\text{init}}$, find their velocities $\mathbf{v}$ and coordinates $\mathbf{r}$ at the next moment $t = t_{\text{next}}$ assuming that the particles interact only through the Newtonian force of gravity. If $\mathbf{r}_i$ and m_i are the coordinates and masses of the particles, then the equations of motion are

$$\frac{d^2 \mathbf{r}_i}{dt^2} = -G \sum_{j=1, i \neq j}^N \frac{m_j (\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3}, \quad (2.8)$$

where G is the gravitational constant. Two steps should be taken before we start solving Eq. (2.8) numerically.

First, we introduce force softening: we make the force weaker (“softer”) at small distances to avoid very large accelerations when two particles collide or come very close to each other. This makes the numerical integration schemes stable. Another reason for softening the force at small distances is that in cosmological environments, when one deals with galaxies, clusters of galaxies, or the large-scale structure, effects of close collisions between individual particles are very small and can be neglected. In other words, the force acting on a particle is dominated by the cumulative contribution of all particles, not by a few close individual companions.

There are different ways of introducing the force softening. For mesh-based codes, the softening is defined by the size of cell elements. For Tree codes, the softening is introduced by assuming a particular kernel, and it is different for different implementations. The simplest and frequently used method is called the Plummer softening. It replaces the distance between particles $\Delta r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ in Eq. (2.8) with the expression $(\Delta r_{ij}^2 + \epsilon^2)^{1/2}$, where ϵ is the softening parameter.

Second, we need to introduce new variables to avoid dealing with too large or too small physical units of a real problem. This can be done in a number of ways. For mesh-based codes, the size of the largest resolution element and the Hubble velocity across the element give scales of distance and velocity. Here, we use more traditional scalings. Suppose M and R are scales of mass and distances. These can be defined by a particular physical problem. For example, for simulations of an isolated galaxy, M and R can be the total mass and the initial radius. It really does not matter what M and R are. The scale of time t_0 is chosen as $t_0 = (GM/R^3)^{-1/2}$. Using M , R , and t_0 , we can change the physical variables $\mathbf{r}_i$, $\mathbf{v}_i$, m_i into dimensionless variables using the following relations:

$$\mathbf{r}_i = \tilde{\mathbf{r}}_i R, \quad \mathbf{v}_i = \tilde{\mathbf{v}}_i \frac{R}{t_0}, \quad m_i = \tilde{m}_i M, \quad t = \tilde{t} t_0. \quad (2.9)$$

We now change the variables in Eq. (2.8) and use the Plummer softening:

$$\tilde{\mathbf{g}}_i = - \sum_{j=1}^N \frac{\tilde{m}_j (\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j)}{(\Delta \tilde{r}_{ij}^2 + \tilde{\epsilon}^2)^{3/2}}, \quad \frac{d\tilde{\mathbf{v}}_i}{d\tilde{t}} = \tilde{\mathbf{g}}_i, \quad \frac{d\tilde{\mathbf{r}}_i}{d\tilde{t}} = \tilde{\mathbf{v}}_i, \quad (2.10)$$

where $\bar{g}_i$ is the dimensionless gravitational acceleration. Note that these equations look exactly as Eq. (2.8) if we formally set $G = 1$ and $\epsilon = 0$.

All numerical algorithms for solving these equations include three steps, which are repeated many times:

- find acceleration: $g(r)$,
- update velocity: $v = v + \Delta v(g)$,
- update coordinates: $r = r + \Delta r(v)$.

Here is a simple fragment of a Fortran-90 code that does it using direct summation of accelerations:

```

Program Simple
  .... (set parameters)
  .... (read data)
  Do                                ! Main loop of integration
    Call Acceleration ! find acceleration for every particle
    v = v+g*dt         ! update velocities
    X = X+v*dt         ! update coordinates
    t = t +dt          ! update time
    If(t> t_end)exit   ! stop when final time is reached
  End do
end Program Simple

Subroutine Acceleration ! find accelerations for each particle
  g = 0.                ! set acceleration to zero for all particles
  Do i=1,N              ! for each particle i
    Do j=1,N            !      add contributions of other particles
      g(:,i)=g(:,i)+m(j)*(X(:,j)-X(:,i))/ &
        sqrt(SUM((X(:,j)-X(:,i))**2+eps2)**3)
    EndDo
  EndDo
end Subroutine Acceleration

```

In this code, we extensively use the Fortran-90's feature of vector operations. For example, the statement $V = V + g \times dt$ means “do it for every element” of arrays $V(i,j)$ and $g(i,j)$. There are simple ways of speeding up the code. Particles can be assigned into groups according to their accelerations with each group having their own time step. In this case, particles with large accelerations update their coordinates and accelerations more often while particles in low density (and acceleration) regions move with large time step, thus reducing the cost of their treatment. Calculations of the acceleration can be easily parallelized using OpenMp directives. These optimizations can speed up the code by hundreds of times, making it a useful tool for simple simulations.

2.4. Moving particles: Time-stepping algorithms

Numerical integration of equations of motion are relatively simple as compared with the other part of the N -body problem — the force calculations. Still, a wrong choice of parameters or an integrator can make a substantial impact on the accuracy of the final solution and on the CPU time. To make arguments more transparent, we write equations of motion in proper coordinates and assume that the gravitational acceleration can be estimated for every particle. In this case, the equations of motion for each particle are simply

$$\frac{d\mathbf{v}(\mathbf{t})}{dt} = \mathbf{g}(\mathbf{x}), \quad \frac{d\mathbf{x}(\mathbf{t})}{dt} = \mathbf{v}(\mathbf{t}). \quad (2.11)$$

Along particle trajectory acceleration can be considered as a function of time $\mathbf{g}(\mathbf{x}(\mathbf{t}))$. If we know coordinates $\mathbf{x}_0$ and velocities $\mathbf{v}_0$ at some initial moment t_0 , then (2.11) can be integrated from $t = t_0$ to $t_1 = t_0 + dt$:

$$\mathbf{x}_1 = \mathbf{x}_0 + \int_{t_0}^{t_1} \mathbf{v}(\mathbf{t}) d\mathbf{t}, \quad \mathbf{v}_1 = \mathbf{v}_0 + \int_{t_0}^{t_1} \mathbf{g}(\mathbf{t}) d\mathbf{t}. \quad (2.12)$$

We now expand $\mathbf{v}(\mathbf{t})$ and $\mathbf{g}(\mathbf{t})$ in the Taylor series around t_0 and substitute those into (2.12) to obtain different approximations for $\mathbf{x}_1$ and $\mathbf{v}_1$. If we keep only the first two terms, we get the first-order Euler approximation: $\mathbf{x}_1 = \mathbf{x}_0 + \mathbf{v}_0 dt + \epsilon$, where $\epsilon \approx g_0 dt^2/2 \propto O(dt^2)$ and $\mathbf{v}_1 = \mathbf{v}_0 + \mathbf{g}_0 dt + \epsilon$, $\epsilon \propto O(dt^2)$. Accuracy and convergence of the Euler integrator are low, and it is never used for real simulations. One may think that adding $g_0 dt^2/2$ term to displacements may increase the accuracy, but it really does not because velocities are still of the first order. In the next iteration, the first-order velocity makes the displacement also of the first order. However, we may dramatically improve the accuracy by rearranging terms in the Taylor expansion in order to kill some high-order terms.

Suppose initial velocity is given not at the moment t_0 , but a half time step earlier at $t_{-1/2} = t_0 - dt/2$. Using coordinates at t_0 , we find acceleration $\mathbf{g}_0(\mathbf{t}_0)$. We now advance velocity one step forward from $t_{-1/2}$ to $t_{1/2} = t_{-1/2} + dt$. Note that when we do it, we use acceleration at the middle of the time step, not on the left boundary of the time step as in the Euler integrator. We then advance coordinates to moment $t_1 = t_0 + dt$ using the new value of velocity. As the result, the scheme of integration is

$$\mathbf{v}_{1/2} = \mathbf{v}_{-1/2} + \mathbf{g}_0 dt, \quad \mathbf{x}_1 = \mathbf{x}_0 + \mathbf{v}_{1/2} dt. \quad (2.13)$$

In order to find the accuracy of this approximation, we first eliminate velocities from (2.13): $\mathbf{x}_1 - 2\mathbf{x}_0 + \mathbf{x}_{-1} = \mathbf{g}_0 dt$. There is an error in this integrator, which we can find by using the Taylor expansion for $\mathbf{x}_{\pm 1}$ up to the fourth-order term. This gives

$$\mathbf{x}_1 - 2\mathbf{x}_0 + \mathbf{x}_{-1} = \mathbf{g}_0 dt + \epsilon, \quad (2.14)$$

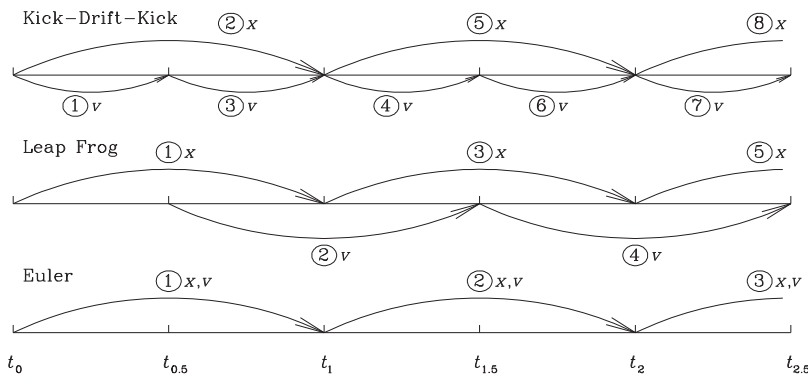


Fig. 2.1. Different schemes for numerical integration of equations of motion. Numbers in circles indicate the sequence of steps in calculating changes in coordinates and velocities with letter following the number showing which parameter — coordinates x or velocities v — is modified. Gravitational acceleration is recalculated after each advance in coordinates.

where the error of the approximation is

$$\epsilon = \frac{1}{12} \frac{d^2 g}{dt^2} dt^4. \quad (2.15)$$

Here, the second time derivative of the acceleration is estimated at $t = t_0$. This is a dramatic improvement as compared with the Euler integrator: the error is proportional to dt^4 and, as a bonus, there is a small factor $1/12$.

In astronomy, the integrator is called the leap frog because velocities are “jumping over” coordinates and then coordinates are “jumping over” velocities. Figure 2.1 shows the sequence of advances of coordinates and velocities for the Euler and leap-frog integrators. Besides being more accurate than the Euler integrator, the leap-frog integrator has two more serious advantages. It is time reversible: if we change the direction of time, flip the direction of velocities and repeat all the steps in the reverse direction, we will arrive at the same initial conditions from which we started (neglecting the rounding errors). This preserves one of the basic properties of the Newtonian equations of motion: time reversibility. Another property is the Hamiltonian structure of the equations of motion. Because we solve the equations only approximately, we introduce errors, that in general may be non-Hamiltonian. These non-Hamiltonian errors in practice result in a gradual change in the total energy of the numerical solution. The leap-frog integrator has a very good property in that its errors are Hamiltonian. In other words, the numerical solution provided by the leap-frog integration has a Hamiltonian structure, but its Hamiltonian is slightly different from the Hamiltonian of the exact solution. Numerical integrators of this type (preserving Hamiltonian structure) are called symplectic. So, a constant-step leap-frog integrator is symplectic. An indication that an integrator is symplectic is the lack of a long-term drift in the energy.

One disadvantage of the leap frog is that velocities and coordinates are defined at different moments of time. It is convenient to split the integrator into smaller steps that allow for synchronization of time moments and are also easier to modify when the time step changes. An algorithm of integration of trajectories can be written as a sequence of operators, which advance particle positions (called drifts) and change velocities (called kicks). Let $K(dt)$ be an operator (kick) that advances velocities by time dt . Applying the operator simply means $K(dt) : \mathbf{v} = \mathbf{v} + \mathbf{g}dt$. Similarly, the drift operator is $D(dt) : \mathbf{x} = \mathbf{x} + \mathbf{v}dt$. We also need to specify the moment when the gravitational acceleration is calculated and the moment when the decision is made to change the time step. So, we use G and S operators to indicate these two moments. For example, a simple constant-step leap-frog integrator can be written as sequence of $GK(dt)D(dt)GK(dt)D(dt)\dots$

Using the K and D operators, we can also write the leap-frog integrator which starts with $\mathbf{x}$ and $\mathbf{v}$ defined at the same moment of time and ends at $t + dt$ moment:

$$\text{KDK: } K(dt/2)D(dt)GK(dt/2)S. \quad (2.16)$$

New accelerations are estimated after advancing coordinates, and the change in the time step dt is made at the end of each time step. The sequence of actions for the KDK integrator is illustrated in the top panel of Fig. 2.1.

Changing the time step may be necessary when particles experience a vast range of accelerations, which is typically the case in high-resolution cosmological simulations. However, changing the time step results in breaking symmetries and reducing the accuracy of the leap-frog integrator. It becomes nontime-reversible and it loses its ability to preserve the energy. There are some ways to restore these properties, but they are complicated and never used in cosmology.

We illustrate the accuracy and the long-term behavior of different integrators by applying them to a simple yet realistic case of the particle motion in a spherical system with density $\rho \propto r^{-2}$ and gravitational potential $\phi = \ln(r)$. This is a good approximation for the density of dark matter halos with the NFW profile around the characteristic “core” radius. We select an eccentric orbit with the ratio of apo- to pericenter 10:1. This is somewhat larger than the typical ratio of 5:1 in the equilibrium NFW profile, but not unusual. Duration of integration is motivated by how many orbits a star or a dark matter particle orbiting the center of the Milky Way galaxy makes over the age of the Universe. It takes the Sun $\sim 3 \times 10^8$ years to make one period. Thus, we get a total of ~ 30 periods of rotation. Assuming a flat rotation curve, a star with radius of 1 kpc will make 300 orbits over the age of the Universe. The number of periods for a star or a dark matter particle is not much different in a dwarf galaxy: velocities are smaller, but so are the distances. Motivated by these numbers, we run tests for few hundred periods. Accuracy of integration also depends on the number of time steps, which we assume to be 10^5 — a realistic estimate for simulations such as Bolshoi. In our tests, we use 500 time steps for one orbital period.

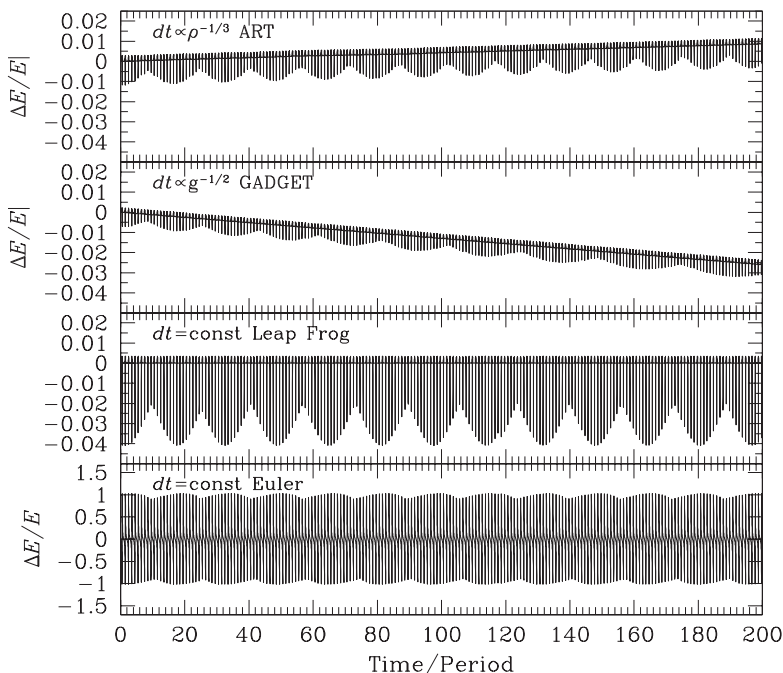


Fig. 2.2. Accuracy of energy conservation for a particle orbiting the center of isothermal density profile $\rho \propto r^{-2}$ in an eccentric orbit with apo- to pericenter ratio 10:1. Trajectories were followed with different integrators, each integrator using 500 time steps per orbital period. The Euler scheme gives the worst accuracy (note the change in the y -axis). The leap frog with a constant time step shows no long-term energy drift, but errors are large as compared with codes with variable time steps. Errors are smaller for variable time step integrators, but they also show a linear trend with time.

Figure 2.2 shows the results obtained with different integrators. The Euler scheme was by far the worst. A constant-step leap-frog integrator is clearly much better: errors are much smaller and they do not grow with time, just as expected for a time-reversible symplectic integrator. However, the errors are still large. The largest error occurs at the smallest radius where the acceleration is the largest. Using an integrator with smaller time step at small radius improves the accuracy as demonstrated by two variable time-step integrators used for the test.

Conditions for changing the time step are different in different codes. For example, in the ART [11] and RAMSES [12] codes, the time step decreases by factor 2 when the number of particles exceeds some specified level (typically 2–6 particles). A cell that exceeds this level is split into eight smaller cells resulting in the drop by 2^3 times of the number of particles in a cell. The time step is also decreased twice. This prescription gives scaling of the time step with the local density ρ as $dt \propto \rho^{-1/3}$. Zemp *et al.* [21] advocate a scheme with scaling of $dt \propto \rho^{-1/2}$. The GADGET [22] and PKDGRAV code use a scaling with the gravitational acceleration $dt \propto g^{-1/2}$, which for $\rho \propto r^{-2}$ gives $dt \propto \rho^{-1/4}$.

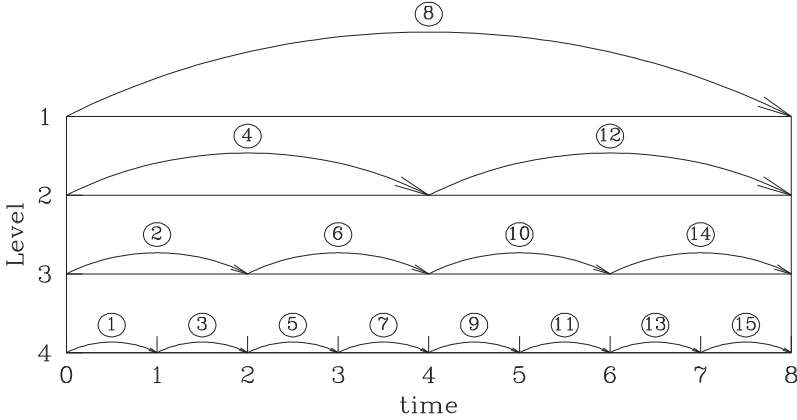


Fig. 2.3. Time-stepping scheme for multilevel resolution codes. In this case, a four-level hierarchy of steps is chosen. Numbers in circles indicate the order of moving particles at different levels.

Results for two variable time-step integrators are presented in two top panels of Fig. 2.2. The first uses the GADGET prescription $dt \propto g^{-1/2}$ and the time step was allowed to change at the end of each time step. Note that in real GADGET runs, the time step changes only by factor 2 when needed. The second variable time-step integrator uses the ART and RAMSES prescription $dt \propto \rho^{-1/3}$. In our particular case, the density changes 10 times along the trajectory. So, the time step changes only once when a particle moves from apocenter to pericenter and once on the way out. The radius of the time-step jump was arbitrarily chosen to be 1/3 of the apocenter radius. Results clearly show improvement in the accuracy but also indicate that errors show systematic drift with time.

Most of the high-resolution N -body codes have particles moving with time steps that differ by a power of 2 from one group of particles to another. The order of advancing different groups and the order of calculation of the gravity force depend on the particular type of code and implementation. Grouping of particles according to force resolution comes naturally in the AMR codes where a particle is assigned to the highest resolution cell that contains the particle. So, the particle takes the attributes of the cell: its size defines the resolution and the time step. In Tree codes, the grouping can be done by particular adopted conditions for the time step refinement. Figure 2.3 gives an example of a sequence of steps in a four-level hierarchy of time steps used in some AMR codes. In this case, we chose a design that attempts to make steps time-symmetric. Quinn *et al.* [23] gave examples of stepping diagrams for a Tree code. A different time-stepping sequence is used in the ENZO code. For example, see [14, Fig. 2].

More detailed discussions of time-stepping in N -body codes can be found in [22–25].

2.5. PM codes

There are a number of advantages of PM codes [3, 7, 8] that make them useful on their own [3, 26–28] or as a component of more complex hybrid Tree-PM codes [22, 29]. Cosmological PM codes are the fastest codes available and they are simple. A PM code solves the Poisson equation (2.4) using a regularly spaced three-dimensional (3D) mesh that covers the cubic domain of a simulation. We start with the calculation of the density field on the nodes of the mesh and then proceed with solving the Poisson equation. Once that is done, the gravitational potential is differentiated to produce acceleration and particles are advanced by one time step.

In order to assign density of particles to the 3D mesh, we introduce a particle shape [7]. If $S(x)$ is the density at distance x from the particle and Δx is the cell size, then the density at distance (x, y, z) is a product $S(x)S(y)S(z)$. Two choices for S are used — Cloud In Cell (CIC) and Triangular Shaped Cloud (TSC):

$$\begin{aligned} \text{CIC: } S(x) &= \frac{1}{\Delta x} \begin{cases} 1, & |x| < \Delta x/2, \\ 0 & \text{otherwise,} \end{cases} \\ \text{TSC: } S(x) &= \frac{1}{\Delta x} \begin{cases} 1 - |x|/\Delta x, & |x| < \Delta x, \\ 0 & \text{otherwise.} \end{cases} \end{aligned} \quad (2.17)$$

The fraction of particle mass assigned to a cell is just a product of three weight functions $w(x)w(y)w(z)$, where $\mathbf{r} = \mathbf{r}_\mathbf{p} - \mathbf{x}_\mathbf{i}$ is the distance between particles with coordinates $\mathbf{x}_\mathbf{p}$ and cell center $\mathbf{x}_\mathbf{i}$, and the weight function is $w(x) = \int_{x_i - \Delta/2}^{x_i + \Delta/2} S(x_p - x') dx'$:

$$\text{CIC: } w(x) = \begin{cases} 1 - |x|/\Delta x, & |x| < \Delta x, \\ 0 & \text{otherwise.} \end{cases} \quad (2.18)$$

$$\text{TSC: } w(x) = \begin{cases} \frac{3}{4} - |x|^2/\Delta x^2, & |x| < \Delta x/2, \\ \frac{1}{2} \left(\frac{3}{2} - |x|/\Delta x \right)^2, & \Delta x/2 < |x| < 3\Delta x/2, \\ 0 & \text{otherwise.} \end{cases} \quad (2.19)$$

Although these relations (2.17)–(2.19) look somewhat complicated, in reality, they require very few operations in a code. For the CIC scheme, a particle contributes to the eight nearest cells. If coordinates are scaled to be from 0 to N_{grid} , where N_{grid} is the size of the grid in each direction, then taking an integer part of each coordinate of particle with center (x, y, z) (in Fortran: $i = \text{INT}(x) \dots$) gives

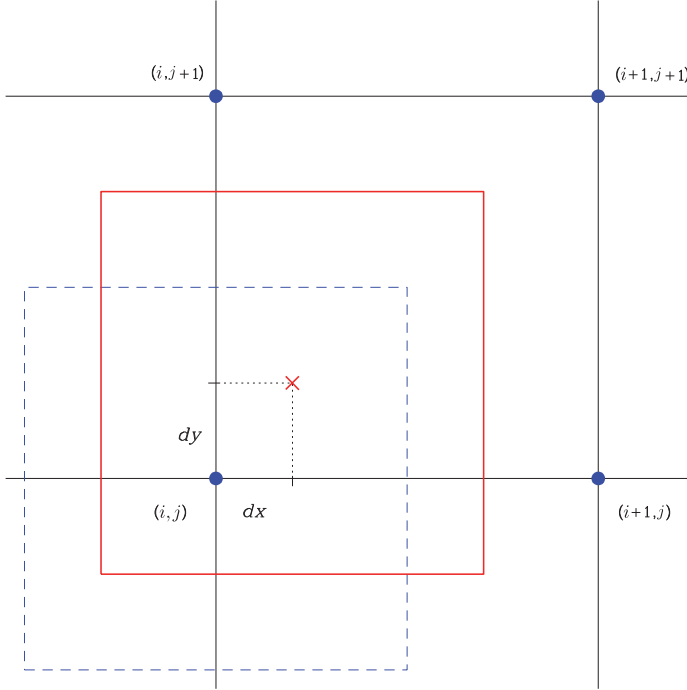


Fig. 2.4. Example of the Cloud-In-Cell density assignment in two dimensions. Centers of mesh cells are shown with large blue circles. Blue dashed square presents boundaries of the cell with coordinates (i, j) . Particle center shown with red cross has coordinates (dx, dy) and its boundaries are shown as red box. Area of intersection of the red and blue boxes is the mass that the particle contributes to the cell (i, j) . All four cells indicated in the plot receive a contribution from the particle.

the lower bottom grid cell (i, j, k) . See Fig. 2.4 for an example in 2D. Then the distance of the particle from that cell center is $dx = x - i, dy = y - j, dz = z - k$. The contributions of the particle to density ρ are

$$\begin{cases} \rho_{i,j,k} = \rho_{i,j,k} + (1 - dx)(1 - dy)(1 - dz) \\ \rho_{i+1,j,k} = \rho_{i+1,j,k} + dx(1 - dy)(1 - dz) \\ \vdots \\ \rho_{i+1,j+1,k+1} = \rho_{i+1,j+1,k+1} + dxdydz. \end{cases} \quad (2.20)$$

Having the density field $\rho_{i,j,k}$, we can estimate the gravitational potential by solving the Poisson equation.

To make the algorithm more transparent, we write the Poisson equation as $\nabla^2 \phi = 4\pi G \rho$. We select the computational volume to be a cube of size L^3 , which is periodically replicated to mimic the Universe. Coordinates of particles are in the limits $0 - L$: if a particle happens to move over a boundary of the cube, it appears

on the other size of the cube. The computational domain is covered by a cubic mesh of size N_{grid}^3 . The mesh is used to store the density field $\rho_{i,j,k}$. The algorithm can be written in such a way that the same mesh is used to store the gravitational potential $\phi_{i,j,k}$. No additional storage is required.

We start with applying a 3D fast Fourier transformation (FFT) to the density field. This gives us Fourier components on a grid of the same size as the density field $\tilde{\rho}_{\mathbf{k}}$, where $\mathbf{k}$ is a vector with integer components in the range $0, 1, \dots, N_{\text{grid}} - 1$. Now, we multiply harmonics $\tilde{\rho}_{i,j,k}$ by the Green functions $G(\mathbf{k})$ to obtain amplitudes of Fourier harmonics of the gravitational potential ϕ :

$$\tilde{\phi}_{\mathbf{k}} = 4\pi G \tilde{\rho}_{\mathbf{k}} G(\mathbf{k}), \quad (2.21)$$

and then do the inverse FFT to find the gravitational potential $\phi_{i,j,k}$. Note that all these operations can be organized in such a way that only one 3D mesh is used.

The simplest, but not the best, method to derive the Green functions is to consider $\phi_{i,j,k}$ and $\rho_{i,j,k}$ as amplitudes of the Fourier components of the gravitational potential in the computational volume and then to differentiate the Fourier harmonics analytically. This gives

$$G_0(\mathbf{k}) = -\frac{1}{\mathbf{k}_x^2 + \mathbf{k}_y^2 + \mathbf{k}_z^2} = -\left(\frac{\mathbf{L}}{2\pi}\right)^2 \frac{1}{\mathbf{i}^2 + \mathbf{j}^2 + \mathbf{k}^2}, \quad (2.22)$$

where $(k_x, k_y, k_z) = (2\pi/L)(i, j, k)$ are components of the wave vector in physical units. A better way of solving the Poisson equation is to start with the finite-difference approximation of the Laplacian ∇^2 . Here, we use the second-order Taylor expansion for the spacial derivatives:

$$\begin{aligned} \nabla^2 \phi &= \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \\ &\approx [\phi_{i+1,j,k} - 2\phi_{i,j,k} + \phi_{i-1,j,k} \\ &\quad + \phi_{i,j+1,k} - 2\phi_{i,j,k} + \phi_{i,j-1,k} \\ &\quad + \phi_{i,j,k+1} - 2\phi_{i,j,k} + \phi_{i,j,k-1}]/\Delta x^2. \end{aligned} \quad (2.23)$$

This approximation leads to a large system of linear algebraic equations: $A\phi = 4\pi G\rho$, where ρ is the vector on the RHS, ϕ is the solution, and A is the matrix of coefficients. All of its diagonal components are equal to -6 , and all six nearest off-diagonal components are 1. The solution of this matrix equation can be found by applying the Fourier transformation. This provides another approximation for the Green functions:

$$G_1(\mathbf{k}) = \frac{\Delta x^2}{2} \left[\cos\left(\frac{2\pi\mathbf{i}}{N_{\text{grid}}}\right) + \cos\left(\frac{2\pi\mathbf{j}}{N_{\text{grid}}}\right) + \cos\left(\frac{2\pi\mathbf{k}}{N_{\text{grid}}}\right) - 3 \right]^{-1}. \quad (2.24)$$

For small (i, j, k) , Eq. (2.24) gives the same results as Eq. (2.21). However, at (i, j, k) close to N_{grid} , the finite-difference scheme G_1 provides less suppression for high-frequency harmonics and thus gives a stronger and more accurate force at distances close to the grid spacing Δx . Hockney and Eastwood [7] argue that this happens because the finite-difference approximation partially compensates damping of short waves related to the density assignment.

The computer memory puts constraints on the PM method because the method requires a large 3D mesh of size N_{grid}^3 while the force resolution increases only as the first power of N_{grid} : $\Delta x = L/N_{\text{grid}}$, where L is length of the computational box. As we start to increase the resolution, we quickly run out of the computer memory.

2.6. AMR codes

We can improve the PM method by increasing the resolution only where it is needed: by placing additional small-size elements — cubic cells — only in regions where there are many particles and where the resolution should be larger. Codes that use this idea are called the adaptive mesh refinement (AMR) codes because they recursively increase the resolution constructing a hierarchy of cubic cells with smaller and smaller elements in dense regions while keeping only large cells in regions that do not require high resolution. There are two ways of doing this: by splitting every element of the mesh, that has many particles, into eight twice smaller boxes [30] or by placing a new rectangular block of cells to cover the whole high density region [31]. ART [11, 32] and RAMSES [12] codes use the first method while ENZO [13] uses the second. Here, we will mostly focus our attention on the method of [30], which is frequently used in cosmological N -body simulations. Here, we mostly follow algorithm and presentation of [11].

Cells are treated as individual units which are organized in refinement trees. Each tree has a root, a cell belonging to a base cubic grid that covers the entire computational volume. If the root is refined (split), it has eight children (smaller nonoverlapping cubic cells residing in its volume), which can be refined in their turn, and so on. Cells of a given refinement level are organized in linked lists and form a refinement mesh. The tree data structures make mesh storage and access in memory logical and simple, while linked lists allow for efficient mesh structure traversals.

The tree ends with unsplit cells, which are called leaves. This structure is called an octal rooted tree and is the construct used in Tree codes. We use fully threaded trees, in which cells are connected with each other on all levels. In addition, cells that belong to different trees are connected to each other across tree boundaries. All cells can be considered as belonging to a single threaded tree with a root being the entire computational domain and the base grid being one of the tree levels. The tree structure is supported through a set of pointers. Each cell has a pointer to its parent and a pointer to its first child. In addition, cells have pointers to the

six adjacent cells (these make the tree fully threaded) so that information about a cell's neighbors is easily accessible.

An elementary refinement process creates eight new cubic cells of equal volume (children) inside a parent cell. When the parent is refined, it is checked if all six neighbors are of the same level as the parent. If there are coarser neighbors (of smaller level than the parent), those neighbors are also split. If a neighbor in its turn has coarser neighbors, the neighbor's neighbors are also split, and so forth. We thus build a refinement structure that obeys a rule allowing no neighbor cells with level difference greater than 1.

Once the refinement structure is built, we can solve the Poisson equation. On the zero (lowest) level, all the volume is covered with a constant-size grid, and the Poisson equation is solved with the FFT method described in Sec. 2.5. The zero-level solution is used on the first refinement level either as an initial guess for the potential of a split cell or as a boundary condition for cells that are not split. After the Poisson equation is solved, the process repeats on the next level.

On each nonzero-level, the Poisson equation is solved using iterative relaxation method [7, 11]. We write the Poisson equation

$$\nabla^2 \phi = \rho \quad (2.25)$$

as a diffusion equation

$$\frac{\partial \phi}{\partial \tau} = \nabla^2 \phi - \rho. \quad (2.26)$$

As the fictitious time τ increases, the initial guess for ϕ approaches (relaxes to) an equilibrium solution, which is the solution of Eq. (2.25). The finite-difference form of Eq. (2.26) is

$$\phi_{i,j,k}^{n+1} = \phi_{i,j,k}^n + \frac{\Delta \tau}{\Delta^2 x} \left(\sum_{l=1}^6 \phi_l^n - 6\phi_{i,j,k}^n \right) - \rho_{i,j,k} \Delta \tau, \quad (2.27)$$

where the summation is over the cell's six neighbors, Δx is the cell size at the current level, and $\Delta \tau$ is fictitious time step. For stability reasons, $\Delta \tau \leq \Delta^2 x/6$. By selecting the maximum allowed time step, we write the iteration scheme as

$$\phi_{i,j,k}^{n+1} = \frac{1}{6} \sum_{l=1}^6 \phi_l^n - \frac{\Delta^2 x}{6} \rho_{i,j,k}. \quad (2.28)$$

The convergence of the relaxation method can be improved in two ways. First, we split all the cells into “black” and “red” such that every “black” cell has only “red” neighbors and vice versa. (One can think about a 3D chess board.) Each iteration is split into two phases: find and replace ϕ only for all “red” cells and then only for “black” ones. Second, one can use the successive overrelaxation (SOR) technique [7].

2.7. Tree and Tree-PM codes

Tree codes [15–19] use different ideas to estimate the force of gravity. Instead of solving the Poisson equation on a mesh as PM and AMR codes do, the Tree codes split particles into groups of different sizes and replace the force from individual particles in the group with a single multipole force of the whole group. The larger the distance from a particle, the bigger the allowed size of the particle group. Modern variants of the Tree algorithm are typically hybrid codes with the long-range force treated by a PM algorithm and the short range handled by a Tree code [22, 29, 33–35]. Thus, there are four components in a Tree code: (1) grouping algorithm, (2) multipole expansion, (3) condition for selecting size of the group (opening angle condition), and (4) splitting the long- and short-distance forces.

Grouping algorithm: The oct tree algorithm is typically used in many Tree codes [18, 22, 35]. If the number of particles in a cell exceeds a specified threshold, it is split into eight small cubic cells. Example of the oct tree is shown in Fig. 2.5. Binary KD trees were used by [17]. In this method, boundaries of rectangular cells are defined by the position of medians of coordinates of particles along each alternating direction. In some cases, cells are quite elongated in KD tree algorithm. This can be mitigated by modifying the grouping algorithm. Gafton and Rosswog [36] proposed the recursive coordinate bisection (RCB) algorithm that splits cells at the center of mass with the direction of the bisecting plane being perpendicular to the direction of the maximum cell size. Indeed, Fig. 2.5 indicates that cells are less elongated in the case of the RCB algorithm, which is used by [29].

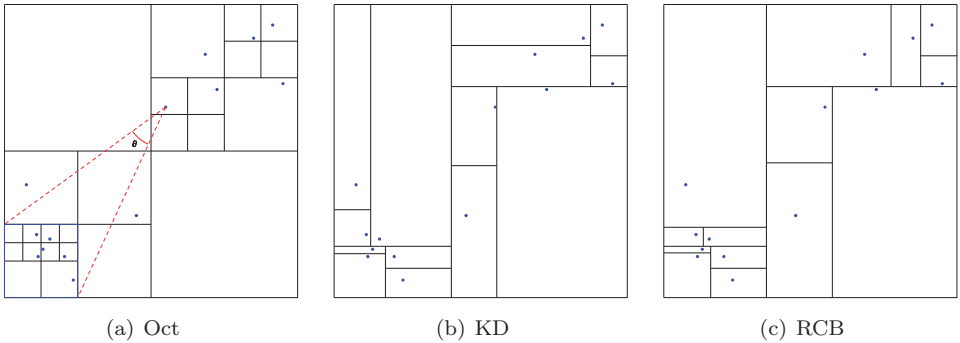


Fig. 2.5. Examples of particle grouping algorithms for Tree codes. *Left panel:* the oct tree for 14 particles presented by blue circles. If the number of particles in a cell exceeds a specified threshold (in this case, one particle), it is split into eight small cubic cells (four cells in 2D). Red dashed lines show opening angle θ for a particles close to the center and for a cell indicated by a thick blue square. *Middle panel:* binary KD tree for the same set of particles. Boundaries of rectangular cells are defined by position of medians along each alternating direction. In some cases, cells are quite elongated. *Right panel:* RCB tree. Cells are split at the center of mass with the direction of the bisecting plane being perpendicular to the direction of the maximum cell size. Cells are less elongated than in the case of KD trees.

Tree is truncated once a cell reaches a specified minimum number of particles. In this case, the cell is called a leaf. The number of particles in a leaf can be as low as one. However, it can be significantly larger [29, 37]. If a leaf has more than one particle, then forces between particles in the cell are estimated using pairwise summation. This can be faster than building more levels of the Tree hierarchy.

Multipole expansion: A number of physical quantities are collected for each cell that are used for force estimates. GADGET-2 code [22] stores the mass and the center of mass of all particles in a given cell. Multipole expansion up to hexadecapole is used in PKDGRAV [17]. Quadrupole expansion was used by [19, 38]. There is no rule on what order of expansion to select. Low orders are faster to calculate and less memory is needed to store the information. At the same time, higher orders of expansion may allow one to use larger opening angles, resulting in faster overall calculations. Grouping algorithm may also affect the selection of the expansion. The bisection trees can produce elongated cells implying that a higher order of mass expansion may be needed to maintain force accuracy.

Cell-opening condition: Once the Tree is constructed and all information regarding mass distribution in each cell is stored, we start to find the forces by looping through all leaves and for each leaf by walking along the Tree down from the largest cells. For each cell of size l , the angle as seen by particles in the leaf at distance d , $\theta \approx l/d$ is tested. If θ exceeds a specified threshold, the force contributions are not taken from the cell itself. We “open” the cell meaning that we descend to children of the cell and test them regarding their opening angles. Once the opening angle is small enough, the force contribution from the cell is accepted, and the algorithm proceeds to the next top-level cell.

Particular implementation of the cell-opening condition changes from code to code. In GADGET-2, the force is accepted if

$$\theta = \frac{l}{d} \leq \sqrt{\alpha g / [GM/d^2]}, \quad (2.29)$$

where g is the particle acceleration from the previous time step, d is the distance from the particle to the cell of mass M and linear size l . Here, α is a tolerance parameter defining the error of the force. There is an additional condition that each coordinate distance between the particle and geometrical cell center should be small:

$$|d_i - c_i| \leq 0.6l, \quad i = 1, 2, 3, \quad (2.30)$$

where d_i and c_i are coordinates of the particle and the cell center. GASOLINE [37] uses opening condition:

$$\theta = \frac{2B_{\max}}{\sqrt{3}d} \leq \alpha, \quad (2.31)$$

where $B_{\max}$ is the maximum distance between the cell's center of mass and a particle in the cell, d is the distance from the particle, for which the force is estimated, to the cell's center of mass, and α is the tolerance parameter.

Splitting the long- and short-distance forces: In order to advance particles from one moment of time to another, we must estimate the total force of gravity acting on each particle. We can split the total force into a smoothly varying part handled by the PM method and a short-range force estimated by the Tree code. For example, we imagine that a point-size particle — a delta function in space — with mass m and position $\mathbf{r}_i$ is split into two components: (1) a sphere S of constant density and radius r_s and (2) the point mass m minus the sphere with mass m . Schematically, we can write the total density as

$$\rho(\mathbf{r}) = \mathbf{S}(\mathbf{r} - \mathbf{r}_i; \mathbf{r}_s, \mathbf{m}) + [m\delta(\mathbf{r} - \mathbf{r}_i) - \mathbf{S}(\mathbf{r} - \mathbf{r}_i, \mathbf{r}_s, \mathbf{m})] \equiv \rho^{\text{PM}} + \rho^{\text{Tree}}. \quad (2.32)$$

If we open the brackets and collect all the terms, we just get the original point mass. Note that the second term in the RHS, ρ^{Tree} , has the total mass equal to zero. So, it does not produce a force at distances $r > r_s$. It can be estimated by a Tree algorithm which is simplified in this case by the fact that we should not look for force contributions from particles and cells which are at a distance larger than r_s . In other words, the *walk* over the tree includes only a local search. This dramatically speeds up the Tree part of the code. The first term ρ^{PM} represents the smooth component of the density distribution and can be efficiently handled by the PM algorithm. This splitting algorithm also simplifies the situation with periodical boundary conditions, which is a complication for pure Tree codes.

In practice, the sphere S may not have a constant density, and the point mass should be replaced by softened density profile. Hockney and Eastwood [7] present details of force splitting used in the historically important P³M code. Here, we follow the prescription for the force splitting in GADGET-2. Another example of force splitting is given by [29]. The gravitational potential ϕ in GADGET-2 is split in Fourier space into two components $\phi_k = \phi_k^{\text{PM}} + \phi_k^{\text{Tree}}$, where the long-distance part ϕ_k^{PM} is obtained with the PM code that has additional filter r_s :

$$\phi_k^{\text{PM}} = \phi_k \exp(-k^2 r_s^2). \quad (2.33)$$

The scale of the filter is larger by a factor 1–3 than the PM cell size. The short-range part of the gravitational potential is estimated in the real space:

$$\phi_k^{\text{Tree}}(\mathbf{x}) = -\mathbf{G} \sum_i \frac{\mathbf{m}_i}{|\mathbf{x} - \mathbf{r}_i|} \text{erfc}\left(\frac{|\mathbf{x} - \mathbf{r}_i|}{2r_s}\right), \quad (2.34)$$

where the summation is taken over all particles and cells that can contribute to the short-range force at $\mathbf{x}$.

2.8. Evolution of the dark matter density and the power spectrum

We review some results of N -body simulations. It is nearly impossible to even mention all important results and to cite all relevant publications — there are too many of them. The goal is to present the main qualitative results and trends of few basic properties of the distribution and evolution of the dark matter: the density distribution function and the power spectrum. Results presented below have been known before. They are reproduced using the publicly available MultiDark and Bolshoi simulations [39–41] and simulations done using the PM code of [42]. All simulations use the Planck cosmological parameters [43].

2.8.1. Dark matter density

At very high redshifts and on very large scales, fluctuations grow close to the predictions of the linear theory. As the amplitude of fluctuations increases, they enter the regime of nonlinear evolution. The transition to the nonlinear regime is complicated and can be roughly split into two stages: weakly and strongly nonlinear.

We start with the evolution of the probability density function (PDF), which tells us what fraction of the volume is occupied by regions with a given density. We randomly place in space a cube of size Δx and measure the mass M inside it and its average density: $\rho = M/\Delta x^3$. What is the probability $p(\rho)d\rho$ that the volume element has density ρ ? This quantity has a long history in cosmology [44–46]. We will discuss PDF for dark matter, but instead we also could analyze, for example, the distribution function of galaxies. This leads us to the statistics called cell counts: how many cells have N objects [47–50].

In the linear regime, the distribution function is a Gaussian:

$$p_{\text{lin}}(\rho) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\delta^2}{2\sigma^2}\right), \quad (2.35)$$

where $\delta \equiv \rho/\rho_m - 1$ is the density contrast, ρ_m is the average density, and σ^2 is the dispersion of δ . As the fluctuations grow, they become nonlinear, and $p(\rho)$ starts to show deviations from the Gaussian distribution. Figure 2.6 shows the evolution of PDF as measured with cells of size $\Delta x = 2.2 h^{-1}\text{Mpc}$. At redshift $z = 20$, the fluctuations are almost in the linear regime and $p(\rho)$ is well approximated by the Gaussian distribution Eq. (2.35). Still, the fit is far from perfect. For example, the peak of $p(\rho)$ is at $\rho < \rho_m$, and there is an excess of cells with large densities. This happens because the fluctuations just start to deviate from the linear growth.

By $z = 4$, the nonlinearities become stronger, which is clearly demonstrated by a very skewed shape of the PDF: the maximum has shifted to even lower densities, and more mass migrated to larger densities. At this weakly nonlinear regime, the PDF can be approximated by the log-normal distribution [44, 46]:

$$p_{\text{log}}(\rho) = \frac{1}{\sqrt{2\pi\sigma^2}} \left(\frac{\rho}{\rho_m}\right)^{-1} \exp\left(-\frac{[\ln(\rho/\rho_m) + \sigma^2/2]^2}{2\sigma^2}\right). \quad (2.36)$$

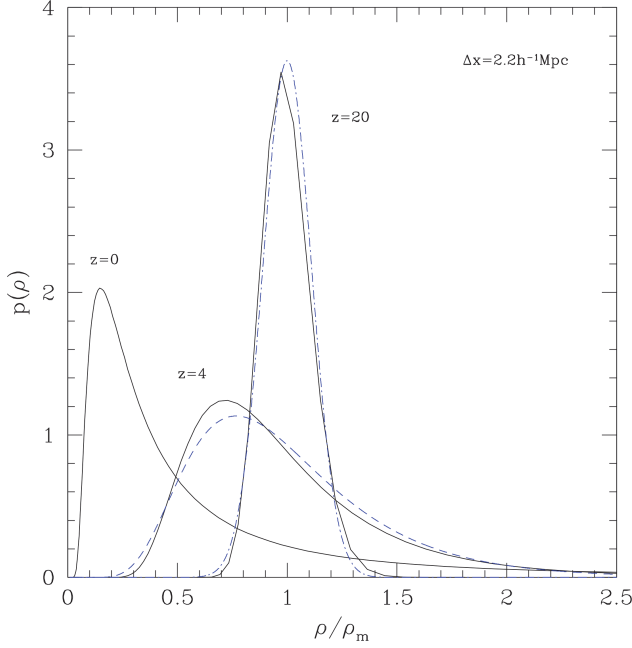


Fig. 2.6. Evolution of the density distribution function with the redshift. The PDF was estimated using cells with size $2.2 h^{-1} \text{Mpc}$. At $z = 20$, the fluctuations at this scale are still almost in the linear regime with the Gaussian distribution (dot-dashed curve) providing a good fit. By $z = 4$, stronger nonlinear effects result in a very skewed distribution with the maximum of $p(\rho)$ shifting to low density and significant enhancement at large densities. At this stage of evolution, $p(\rho)$ can be approximated by the log-normal distribution (dashed curve). However, it starts to badly fail for later stages of evolution.

When the fluctuations become strongly nonlinear, the PDF develops a very long tail at large densities while its maximum shifts to even lower densities. Figure 2.7 shows $\rho p(\rho)$ at different moments. Here, we use a small cell size of $\Delta x = 1.1 h^{-1} \text{Mpc}$ that also allows us to probe fluctuations with larger densities. At $z = 4$, the log-normal distribution still provides a fit for data around the maximum of PDF, but it fails at the wings. At $z = 0$, the log-normal distribution becomes nearly useless: it fails practically everywhere.

At this strongly nonlinear regime, the distribution function $p(\rho)$ develops a nearly power-law shape with an exponential decline:

$$p(\rho) \propto \rho^{-2} \exp(-\alpha \rho^{3/4}), \quad \rho > 10 \rho_m. \quad (2.37)$$

Figure 2.7 shows that this provides a very good approximation to the data.

Figure 2.8 shows the evolution of the dark matter power spectrum and demonstrates the three regimes of growth of fluctuations [51–53]:

- (1) On large scales (small k), the fluctuations grow according to the predictions of the linear theory. Here, the shape of the power spectrum $P(k, z)$ does not

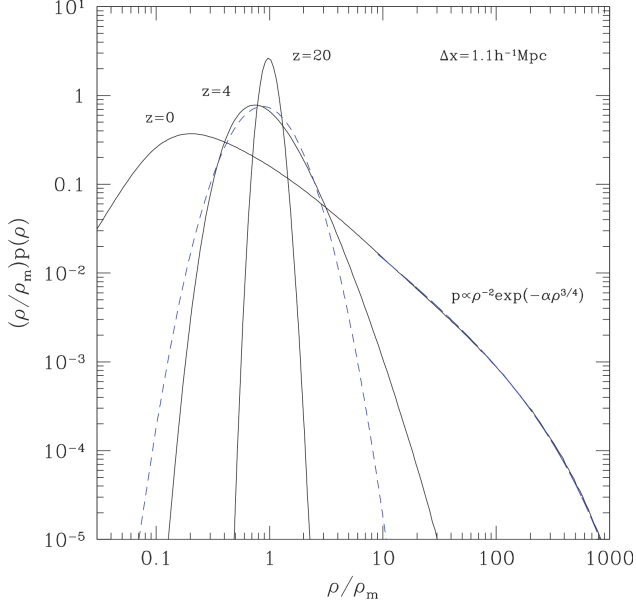


Fig. 2.7. Detailed view of the density distribution function. PDF is scaled with the density and plotted on the logarithmic scale. A small cell of $1.1 h^{-1} \text{Mpc}$ is used. At $z = 4$, the log-normal distribution substantially deviates from the data at both low and large densities, but gives a sensible fit close to the maximum. At $z = 0$, the distribution function is so asymmetric that it cannot be even remotely approximated by the log-normal distribution. At large densities, $p(\rho)$ is accurately approximated by a power law with an exponential decline.

change, but its amplitude increases with time: $P(k, z) = D^2(z)P_{\text{lin}}(k)$, where $D(z)$ is the linear growth factor normalized to be unity at present $D(z = 0) = 1$, and $P_{\text{lin}}(k)$ is the linear power spectrum.

- (2) On smaller scales (larger k), the fluctuations enter a weakly nonlinear regime where the amplitude of fluctuations is still relatively small, but the fluctuations grow substantially faster than in the linear regime. The scale at which the fluctuations start to show a nonlinear trend evolves with time. As time increases, the wave number of the transition k_{NL} becomes smaller and the amplitude $P(k_{\text{NL}})$ increases. The exact value of k_{NL} is somewhat arbitrary. If we choose the point at which $P(k)$ is, say 20%, larger than the linear theory, then $k_{\text{NL}} \approx 0.2 h \text{Mpc}^{-1}$ at $z = 0$ and $k_{\text{NL}} \approx 1 h \text{Mpc}^{-1}$ at $z = 5.5$.
- (3) On even smaller scales, the fluctuations become strongly nonlinear and enter the regime of stable clustering. Contrary to naive expectations, the rate of the nonlinear evolution is the fastest in the weakly nonlinear regime. In strongly nonlinear regime, the dark matter is mostly in collapsed and nearly virialized halos. The halos still accrete mass and grow, but most of this mass stays in the outer halo regions. The inner regions of the halos preserve their proper radius and mass (hence the name “stable clustering”). Assuming that the number of

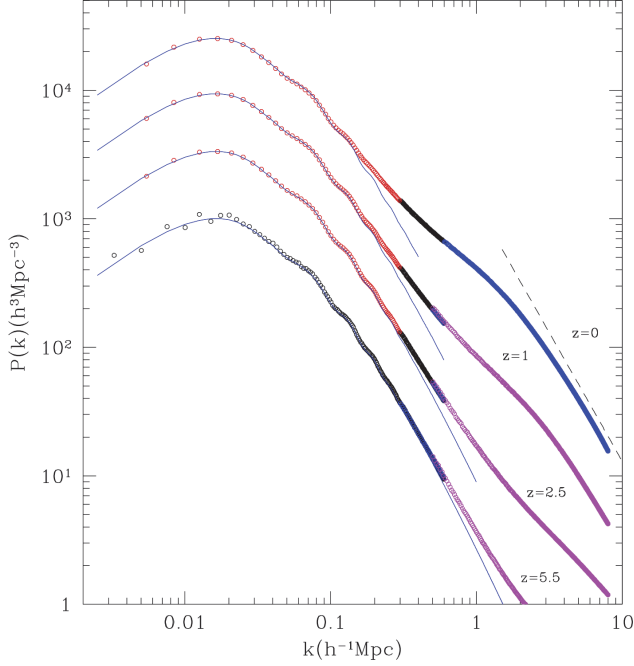


Fig. 2.8. Evolution of the dark matter power spectrum. Simulations with different computational boxes and resolutions are shown by circles with different colors. Blue curves show predictions of the linear theory. The plot shows that at any redshift, the power spectrum $P(k)$ has three regimes of growth: (1) linear growth on very long waves (small $k \lesssim 0.1 h\text{Mpc}^{-1}$) followed on larger wavenumbers by (2) the weakly nonlinear regime where fluctuations grow much faster than predictions of the linear theory, and (3) strongly nonlinear evolution at $k \gtrsim 1 h\text{Mpc}^{-1}$. In this regime, the power spectrum gradually approaches power law $P(k) \propto k^{-2}$ shown as the dashed line in the plot.

pairs with a given proper separation r is preserved, the only effect, which is left, is the shrinking of halos in the comoving coordinates $x = r/a$. This leads to the increase in the power spectrum $P(k') \propto a^3$ and to the increase of the wavenumber $k' = ak$ [53, 54]. In the $P(k, z) - k$ plane, points start to drift to the right along k -axis and upward along P -axis as the fluctuations enter the stable clustering regime.

There are different ways to make analytical predictions for the nonlinear evolution of the power spectrum. Hamilton *et al.* [55] were the first to propose a physically motivated phenomenological model of mapping the linear correlation function $\xi_{\text{lin}}(r) \propto a^2$ into the nonlinear function $\xi(r')$ by assuming a transition from the linear regime where $\xi = \xi_{\text{lin}} \propto a^2$ and $r' = r$ to the regime of stable clustering where $\xi(r') = a\xi_{\text{lin}} \propto a^3$ and $r'^3 = (1 + \Delta_{\text{NL}}^2)r'^3$, where Δ_{NL}^2 is the nonlinear estimate of the amplitude of fluctuations on the scale r' . Later, Peacock and coworkers [51–53] improved the model, which works reasonably well providing $\sim 10\%$ level of accuracy [56, 57]. This may not be accurate enough for some tests. However, the

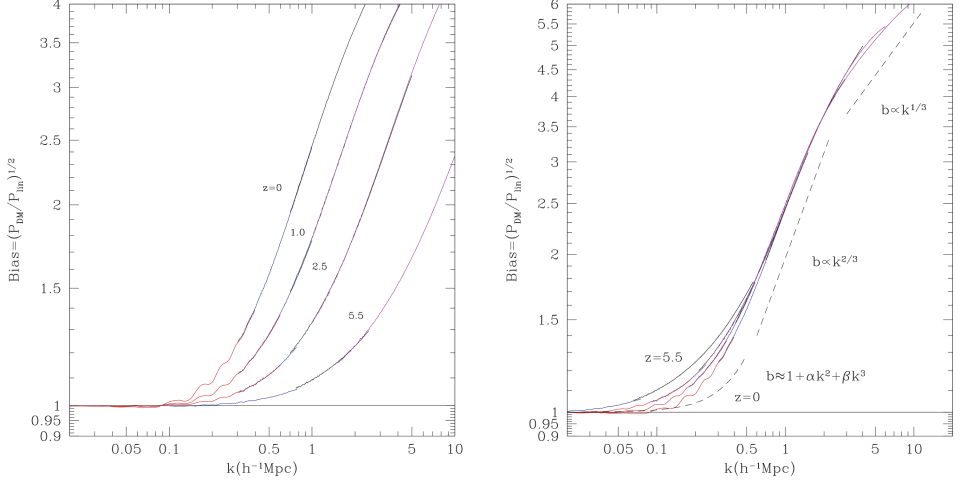


Fig. 2.9. *Left panel:* Dependence of the bias parameter $b = \sqrt{P_{DM}(k)/P_{linear}(k)}$ on the wavenumber and redshift. Wiggles at $k \sim (0.1 - 0.3) h^{-1}\text{Mpc}$ are related to the smearing of the BAO oscillations by the nonlinear interactions. *Right panel:* Bias parameter rescaled to have the same k at $b = 2$. The plot illustrates self-similar growth of perturbations in the strongly nonlinear regime $b \gtrsim 2$.

model has an advantage that it provides a sensible approximation even at very large k where no other approximation works. It also gives qualitative explanation of the very nonlinear regime.

There is a different way of looking at the evolution of the power spectrum. Instead of plotting $P(k)$ at different redshifts, we can study the evolution of the ratio of the power spectrum P to the prediction of the linear theory P_{lin} . This quantity is called the dark matter bias:

$$b^2(k; z) \equiv \frac{P(k; z)}{P_{lin}(k; z)}. \quad (2.38)$$

Left panel in Fig. 2.9 shows the evolution of the bias $b(k; z)$ for the ΛCDM model with the Planck cosmological parameters. At any redshift, there is a region at low wavenumbers k where $b \approx 1$. This is the domain of the linear growth of fluctuations. At larger k , the bias factor starts to increase first as $k \approx 1 + \alpha(z)k^2$, where $\alpha(z)$ is a function of time. Then at larger k , the bias factor deviates from this simple shape.

At $k \sim (0.1 - 0.3) h^{-1}\text{Mpc}$, there are wiggles in the bias parameter that grow over time. Those wiggles are associated with the baryonic acoustic oscillations (BAO) [58, 59]. BAOs are related to the propagation of acoustic waves in the primordial plasma before the epoch of recombination $z \approx 1000$. During the recombination, there is a sudden drop in the gas pressure and sound speed, which in turn effectively terminates the propagation of the acoustic waves. The characteristic scale of the acoustic horizon at the moment of recombination translates into a peak in the correlation function at $\sim 110 h^{-1}\text{Mpc}$ for the standard cosmology. (The exact

value depends on cosmological parameters Ω_m, Ω_b , and h .) The Fourier transform of the peak in the correlation function produces wiggles in the power spectrum of perturbations. As the perturbations enter the nonlinear regime, the peaks and troughs in $P_{\text{lin}}(k)$ start to be smeared out. This is observed as appearance of wiggles in $b(k)$ in the weakly nonlinear regime.

It is interesting to study the shape of the bias parameter at large wavenumbers. In order to clarify the situation, we rescale $b(k)$ functions at different redshifts to have the same value of k at $b \approx 2$. This is done by scaling k while keeping the bias parameter unchanged: $b(k\beta(z))$, where $\beta(z)$ is a factor that monotonically decreases with the redshift and $\beta(0) = 1$. The right panel in Fig. 2.9 presents the rescaled bias parameter. It shows that the bias parameter at large values $b \gtrsim 2$ evolves in a self-similar fashion: as fluctuations evolve, the same shape of $b(k)$ simply shifts to smaller and smaller wavenumbers. In the limit of very large k , the initial power spectrum scales as $P_{\text{lin}}(k) \propto k^{-3}$ and in the strong nonlinear regime $P(k) \propto k^{-2}$. So, the bias parameter should increase as $b \propto k^{1/2}$. At $k = (3 - 10) h^{-1} \text{Mpc}$ (the largest k in Fig. 2.9), the initial power spectrum is slightly shallower with $P_{\text{lin}}(k) \propto k^{-2.6}$, which gives $b \propto k^{1/3}$, which is what we see in the simulations.

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Chapter 3

Hydrodynamic Methods for Cosmological Simulations*

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Currently, various cosmological and astrophysical experiments are planned or under way mapping a large number of cosmological objects from galaxies to galaxy clusters in unprecedented high precision to understand their dynamical structure in detail and to constrain their formation history and the involved physical processes. Exploiting these datasets is a challenging task. The physics at play, namely, the large-scale gravitational instability coupled to complex galaxy formation physics, is highly nonlinear and some aspects are still poorly understood. To capture the complexity of galaxy formation in a cosmological context, advanced computer simulations have to be performed. Therefore, it is needed to incorporate a variety of physical processes in the calculations, including three that are considered particularly important for the development of the visible universe: first, the condensation of matter into stars, second, their further evolution when the surrounding matter is heated by stellar winds and supernova explosions, and enriched with chemical elements, and third, the feedback of supermassive black holes that eject massive amounts of energy into the universe. In this chapter, we briefly describe the hydrodynamic methods used in cosmological simulations and the most common techniques used to include these processes.

3.1. Introduction

To a first approximation, one can study the formation of cosmic structures using N -body simulations which basically follow the evolution of collisionless particles under gravity. Such simulations have been performed with high resolution for individual objects, like galaxies and galaxy clusters as well as for very large-scale

*This is based on a previous publication of the author [1].

structures, using numerical methods described in Chapter 2. However, with the possible exception of gravitational lensing, observations mainly reflect the state of the ordinary (baryonic) matter. Therefore, their interpretation in the framework of cosmic evolution requires that we understand the complex, nongravitational, physical processes which determine the evolution of the cosmic baryons. The evolution of each of the underlying building blocks (see Video 1, page xiii) — where the baryons fall into the potential well of the underlying dark matter distribution, cool, and finally condense to form stars — within the hierarchical formation scenario will contribute to the state and composition of the intergalactic and intracluster media (IGM and ICM, respectively), and is responsible for energy and metal feedback, magnetic fields, and high-energy particles. Depending on their origin, these components will be blown out by jets, winds or ram pressure effects and finally mix with the surrounding IGM/ICM. Some of these effects will be naturally followed within hydrodynamic simulations (like ram pressure effects), others have to be included in simulations via effective models (like star formation and related feedback, and chemical pollution by supernovae).

Thanks to the improved computing power and advancements in numerical methods, the number of resolution elements¹ which can be utilized in such simulations has increased dramatically over the last 20 yrs as shown in Fig. 3.1. Note that the largest, hydrodynamical simulation up to date (see Video 2, page xiii) [28] followed a total number of more than 2×10^{11} particles (e.g., dark-matter, gas, stars and black hole tracer particles) over the whole evolution of the universe.

In this chapter, we will discuss the basic numerical methods which are used for studying these processes in the context of cosmological simulations (see Video 3, page xiii). Further components like magnetic fields and high-energy particles need additional modeling of their injection processes and evolution. To do so, they must be self-consistently coupled with the hydrodynamics and are described in more detail in Chapter 9.

3.2. Basic hydrodynamical simulations

Given that halos are nonlinear collapsed systems, numerical simulations are the method of choice for theoretical studies. Modern cosmological simulation codes based on N -body and hydrodynamics techniques are capable of accurately following the dynamics of dark matter and gas in their full complexity during the hierarchical build-up of structures.

3.2.1. Basic equations and techniques

The baryonic content of the Universe can typically be described as an ideal fluid, described by a set of equations, namely, the *Euler equations* which consist of the

¹Note that, to be consistent between different simulation techniques, we define resolution elements here as only the number of dark-matter particles not the total number of particles or cells, which would be typically a factor 2 larger.

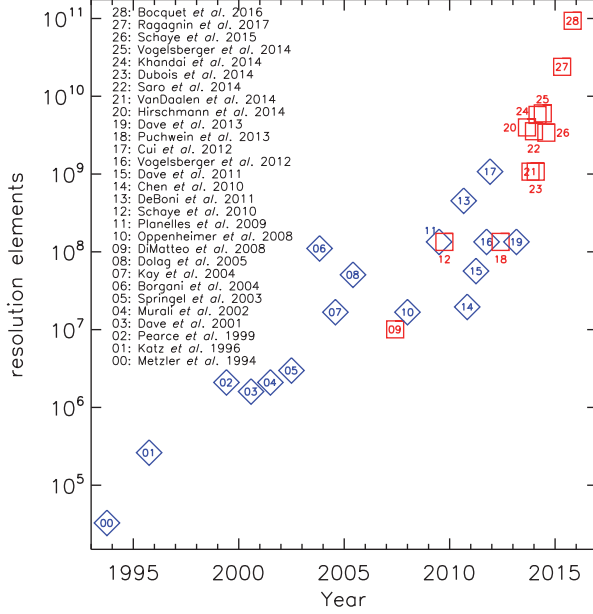


Fig. 3.1. The evolution of the number of resolution elements in hydrodynamical, cosmological simulations over the last two decades. The blue data points are simulations including the effect of cooling and star formation [2–17], the red data points are simulations which in addition include the effect of AGN feedback [18–29].

momentum equation, the *continuity equation*, and the *first law of thermodynamics*:

$$\frac{d\vec{v}}{dt} = -\frac{\vec{\nabla}P}{\rho} - \vec{\nabla}\Phi, \quad (3.1)$$

$$\frac{d\rho}{dt} + \rho\vec{\nabla}\vec{v} = 0, \quad (3.2)$$

$$\frac{du}{dt} = -\frac{P}{\rho}\vec{\nabla} \cdot \vec{v} - \frac{\Lambda(u, \rho)}{\rho}. \quad (3.3)$$

They are closed by an *equation of state*, relating the pressure P to the internal energy (per unit mass) u and the density ρ . Assuming an ideal, monoatomic gas, this will be

$$P = (\gamma - 1)\rho u \quad (3.4)$$

with the polytropic index $\gamma = 5/3$. As result of applying these equations to cosmological structure formation, there are several features emerging in comparison to other, typical, hydrodynamic simulations. First, one has to account for the otherwise often neglected self-gravity, emerging as the $\vec{\nabla}\Phi$ term, which can be solved following the methods described in Chapter 2. Second, radiative losses $\Lambda(u, \rho)$ as laid out in Section 3.4 play a key role in influencing the evolution of the baryonic component,

especially for characterizing the formation of the stellar component within the universe, as outlined in Section 3.5. Additionally, the equations have to be adapted to the cosmological background (e.g., expansion history of the universe).

As a result of the high nonlinearity of gravitational clustering in the Universe, an enormous dynamic range in space and time has to be captured. For instance, the range of hierarchical structures range from sub-kpc scales in galaxies up to several hundreds of megaparsecs, characterizing the largest coherent scale in the Universe.

A variety of numerical schemes for solving the coupled system of collisional baryonic matter and collisionless dark matter have been developed in the past decades. They fall into two main categories: particle methods, which discretize mass (see [30] and references therein) and grid-based methods, which discretize space (see [31] and references therein). Recently, however, various schemes have been developed which combine characteristics of both methods (see [32] and references therein).

3.2.2. Classical Eulerian (grid) methods

In an expanding Universe, where $a(t)$ describes the scale factor of the Universe (normalized to $a = 1$ today), the *Euler equations* read

$$\frac{\partial \vec{v}}{\partial t} + \frac{1}{a}(\vec{v} \cdot \vec{\nabla})\vec{v} + \frac{\dot{a}}{a}\vec{v} = -\frac{1}{a\rho}\vec{\nabla}P - \frac{1}{a}\vec{\nabla}\Phi, \quad (3.5)$$

$$\frac{\partial \rho}{\partial t} + \frac{3\dot{a}}{a}\rho + \frac{1}{a}\vec{\nabla} \cdot (\rho\vec{v}) = 0, \quad (3.6)$$

and

$$\frac{\partial}{\partial t}(\rho u) + \frac{1}{a}\vec{v} \cdot \vec{\nabla}(\rho u) = -(\rho u + P) \left(\frac{1}{a}\vec{\nabla} \cdot \vec{v} + 3\frac{\dot{a}}{a} \right), \quad (3.7)$$

respectively, where the RHS in the last equation reflects the expansion in addition to the usual PdV work.

Grid-based methods solve these equations based on structured or unstructured grids, representing the fluid. One distinguishes *primitive variables*, which determine the thermodynamic properties (e.g., ρ , $\vec{v}$, or P) and *conservative variables* which define the conservation laws (e.g., ρ , $\rho\vec{v}$, or ρu). Early attempts were made using a central difference scheme, where fluid is only represented by the centered cell values and derivatives are obtained by the finite-difference representation (see, for example, [33]). Such methods will however break down in regimes where discontinuities appear. These methods therefore use artificial viscosity to handle shocks (similar to the smoothed particle hydrodynamics method described in Section 3.2.4). Also, by construction, they are only first-order accurate.

Classical approaches use reconstruction schemes, which, depending on their order, take several neighboring cells (so-called *stencils*) into account to reconstruct the field of any hydrodynamical variable with increasing order of accuracy. Typical schemes are *piecewise constant method* (PCM), *piecewise linear method* (PLM; e.g.,

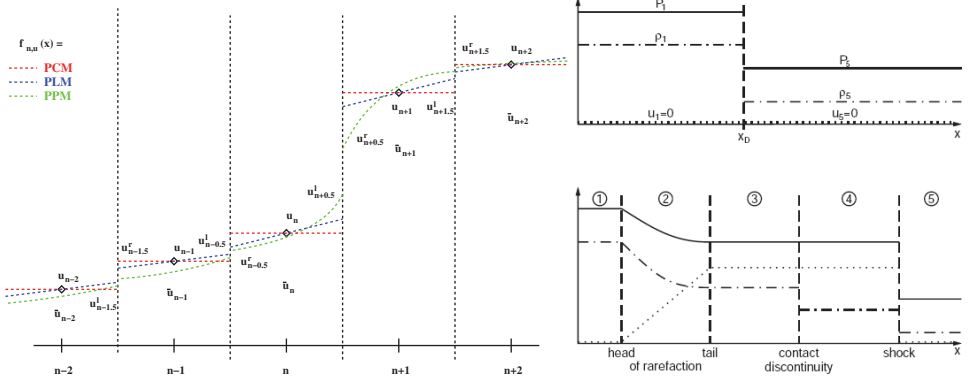


Fig. 3.2. Left panel: Reconstruction of the principal variables (u_n) on the grid using different methods like *piecewise constant* (PCM), *piecewise linear* (PLM), or *piecewise parabolic* (PPM). The reconstruction scheme then allows one to calculate cell averages ($\bar{u}_n$) as well as the left and right-hand side values on the cell boundaries ($u_{n\pm 0.5}^l, u_{n\pm 0.5}^r$). Figure taken from [1]. Right panel: The initial state of the so-called *Riemann problem* (upper panel) and its evolved state (lower panel) for the case of no relative motion between the two sides ($u_1 = u_2 = 0$). The solid lines mark the pressure P , the dashed dotted lines the density ρ and the dotted line the velocity v . Kindly provided by Ewald Müller.

[34]) and *piecewise parabolic method* (PPM [35]), see illustration in the left part of Fig. 3.2. The shape of the reconstruction function is then used to calculate the total integral of a quantity over the grid cell, divided by the volume of each cell (e.g., *cell average*) rather than pointwise approximations at the grid centers (e.g., *central variables*). Modern, high-order schemes usually have *stencils* based on at least five grid points and implement *essentially nonoscillatory* (ENO [36]) or the so-called *weighted essentially nonoscillatory* (WENO [37]) schemes for reconstruction which maintain high-order accuracy (e.g., see [38] for a recent review).

The reconstructed quantities are then used to calculate the left- and right-hand side values at the cell boundaries which are used later as initial conditions to solve the so-called *Riemann problem* (see right panel of Fig. 3.2) whose solution provides the fluxes of various quantities (e.g., mass, energy, etc.) across the cell borders. To avoid oscillations in such reconstructions (e.g., the development of new extrema), additional constraints are included in the reconstruction: the so-called *slope limiters* which estimate the maximum slope allowed for the reconstruction. One way is to demand that the total variation among the interfaces does not increase with time. Such so-called *total variation diminishing* schemes (TVD [39]) nowadays provide various different slope limiters suggested by different authors.

How to solve the general *Riemann problem*, e.g., the evolution of a discontinuity initially separating two states, can be found in textbooks (e.g., [40]). Here, we want to give only a brief description of the solution of a shock tube as one example. This corresponds to a system where both sides are initially at rest. Figure 3.2 shows in the right panel the initial (upper panel) and the evolved (lower panel) systems. The

latter can be divided into five regions. The values for Regions 1 and 5 are identical to the initial configuration. Region 2 is a rarefaction wave which is determined by the states in Regions 1 and 3. The solution can be obtained by invoking the general *Rankine–Hugoniot* conditions, describing the jump conditions at a discontinuity, which read

$$\rho_l v_l = \rho_r v_r, \quad (3.8)$$

$$\rho_l v_l^2 + P_l = \rho_r v_r^2 + P_r, \quad (3.9)$$

$$v_l(\rho_l(v_l^2/2 + u_l) + P_l) = v_r(\rho_r(v_r^2/2 + u_r) + P_r), \quad (3.10)$$

where we have assumed a coordinate system which moves with the shock velocity v_s . Combining such conditions and defining the initial density ratio $\lambda = \rho_1/\rho_5$, one gets the nonlinear, algebraic equation

$$\frac{\rho_1}{\rho_5} \frac{1}{\lambda} \frac{(1-P)^2}{\gamma(1+P) - 1 + P} = \frac{2\gamma}{(\gamma-1)^2} \left[1 - \left(\frac{P}{\lambda} \right)^{(\gamma-1)/(2\gamma)} \right]^2 \quad (3.11)$$

for the pressure ratio $P = P_{3,4}/P_5$. Once $P_{3,4}$ is known by solving this equation, the remaining unknowns can be inferred step by step from the four conditions.

Solving the full *Riemann* problem in a hydrodynamics code can be expensive and severely affect the performance. Therefore, there are various approximate methods to solve the *Riemann* problem, including the so-called *ROE method* (e.g., [41]), the *HLL/HLLE* method (e.g., see [42–44]), and *HLLC* (e.g., see [45]). A description of all these methods is outside the scope of this review, so we redirect the reader to the references given or textbooks like Ref. 46.

A wide variety of codes are used for cosmological applications, including the *TVD*-based codes like those of [47], *CosmoMHD* [48], the *PLM*-based codes (*ART*, [49, 50]), and *RAMSES* [51]. The *PPM*-based codes include those of *Zeus* [52], *ENZO* [53], *COSMOS* [54], and *FLASH* [55]. There is also the *WENO*-based code by [56].

3.2.3. Adaptive mesh refinement

To enlarge the dynamical range of the numerical schemes, mesh refinement strategies have been applied in most grid codes (e.g., *ART*, *RAMSES*, *ENZO*, and *FLASH*). In most of the cases, a simple density (e.g., mass per cell) criterion is used. If the mass within one cell exceeds a certain threshold,

$$m \equiv \rho \Delta x^3 > m_{\min}, \quad (3.12)$$

the cell is divided in multiple (e.g., eight) subcells and the internal properties are interpolated from the original cell onto the new subcells. This ensures that within the computational domain, the gravitational mass (e.g., the source of gravity) is homogeneously distributed. Thereby the underlying grid evolves in a quasi-Lagrangian

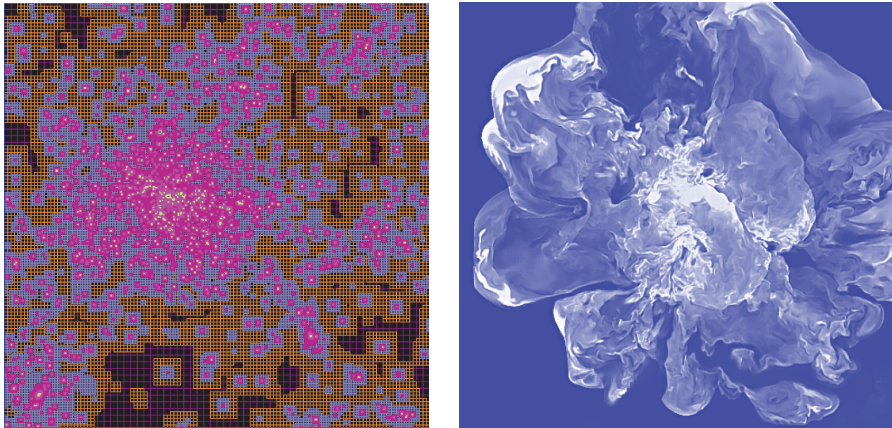


Fig. 3.3. Left panel: Mesh refinement levels of *RAMSES* for a typical, cosmological simulation. Kindly provided by Romain Teyssier. Right panel: Slice in gas temperature through a cluster simulation with refinement based on velocity jumps, therefore unusually high resolution is obtained around shocks even in the outer parts of the cluster. Figure taken from [57].

fashion, following the flow of mass, as can be seen in the left part of Fig. 3.3 which shows the typical structure of the refinement grid in a cosmological simulation.

Note that for studying shocks and turbulence in galaxy clusters, other refinement strategies based on velocity criteria are often used [57, 58]. By extending the standard refinement criteria to additionally refining on velocity jumps, the formation of turbulence and shocks can be followed with unprecedented high spatial resolution throughout the cosmic structures, see right part of Fig. 3.3. In order to follow the turbulent cascade in high precision, subscale turbulence models can additionally be used to initialize the velocities on the refined cells because otherwise the turbulent cascade can be suppressed [59].

3.2.4. Classical Lagrangian (particle) methods

The classical Lagrangian method is the so-called Smoothed Particle Hydrodynamics method (SPH, [60, 61]) which solves the Lagrangian form of the Euler equations and can achieve good spatial resolutions in high-density regions but less well in low-density regions. It also suffers from degraded resolution in shocked regions due to the introduction of a sizeable artificial viscosity. In its classical implementation, discretization errors introduce spurious pressure forces on particles in regions with steep density gradients in particular near contact discontinuities. This results in a boundary gap of the size of an SPH smoothing kernel radius over which interactions are severely damped. The standard implementation typically does not involve an explicit mixing term, which can compensate this effect. Therefore, the classical implementation does not resolve and treat dynamical instabilities in the interaction of multi-phase fluids, such as *Kelvin–Helmholtz* or *Rayleigh–Taylor* instabilities.

Both these shortcomings can be overcome by a modern implementation as described at the end of this section. In addition, in the cosmological context, the adaptive nature of the SPH method, its simple way to couple to gravity and the possibility to have individual time steps often compensate for such shortcomings, thus making SPH still one of the most commonly used methods in numerical hydrodynamical cosmology.

The basic idea of SPH is to discretize the fluid by mass elements (e.g., particles), rather than by volume elements as in Eulerian methods. Therefore, it is immediately clear that the mean interparticle distance in collapsed objects will be smaller than in underdense regions. The scheme will thus be adaptive in spatial resolution by keeping the mass resolution fixed. For a comprehensive review, see [30]. To build continuous fluid quantities for an arbitrary variable X , one starts with a general definition of a kernel smoothing method

$$\langle X(\vec{x}) \rangle = \int W(\vec{x} - \vec{x}', h) X(\vec{x}') d\vec{x}', \quad (3.13)$$

which requires that the kernel is normalized (i.e., $\int W(\vec{x}, h) d\vec{x} = 1$) and collapses to a delta function if the smoothing length h approaches zero, namely, $W(\vec{x}, h) \rightarrow \delta(\vec{x})$ for $h \rightarrow 0$. The kernel should additionally be monotonic and differentiable.

One can write down the continuous fluid quantities (e.g., $\langle X(\vec{x}) \rangle$) based on the discretized values X_j represented by the set of the individual particles m_j at the position $\vec{x}_j$ as

$$\langle X_i \rangle = \langle X(\vec{x}_i) \rangle = \sum_j \frac{m_j}{\rho_j} X_j W(\vec{x}_i - \vec{x}_j, h), \quad (3.14)$$

where we assume that the kernel depends only on the distance modulus (i.e., $W(|\vec{x} - \vec{x}'|, h)$) and we replace the volume element of the integration, $d\vec{x} = d^3x$, with the ratio of the mass and density m_j/ρ_j of the particles. Although this equation holds for any position $\vec{x}$ in space, we are only interested here in the fluid representation at the original particle positions $\vec{x}_i$, which are the only locations where we will need the fluid representation later on. It is important to note that for kernels with compact support (i.e., $W(\vec{x}, h) = 0$ for $|\vec{x}| > h$), the summation does not have to be done over all the particles but only over the particles within the sphere of radius h , namely, the neighbors around the particle i under consideration. Traditionally, the most frequently used kernel is the B_2 -Spline, but modern schemes invoke an entire new family of kernels like the HOCT kernels [62] or the so-called Wendland kernels [63] which show better stability and higher accuracy (see also recent review by [64] and references therein).

When one identifies X_i with the density ρ_i , ρ_j cancels out on the right hand side of Eq. (3.14), and we are left with the density estimate of particle i ,

$$\langle \rho_i \rangle = \sum_j m_j W(\vec{x}_i - \vec{x}_j, h). \quad (3.15)$$

Derivatives can be calculated and pairwise symmetric formulations can be obtained making use of the identity $(\rho \vec{\nabla}) \cdot X = \vec{\nabla}(\rho \cdot X) - \rho \cdot (\vec{\nabla} X)$. Usually, the smoothing length h will be allowed to vary for each individual particle i and is determined by finding the radius h_i of a sphere which contains n neighbors or contains a certain mass.

In general, once every particle has its own smoothing length, a symmetric kernel $W(\vec{x}_i - \vec{x}_j, h_i, h_j) = \bar{W}_{ij}$ has to be constructed (e.g., for additional terms like the artificial viscosity) to keep the conservative form of the formulations of the hydrodynamical equations. Starting from an entropy formulation, [65] for the first time derived an SPH formulation including the proper correction terms for the varying smoothing length from a Lagrangian formalism, obtaining

$$\frac{d\vec{v}_i}{dt} = - \sum_j m_j \left(f_j \frac{P_j}{\rho_j^2} \vec{\nabla}_i W(\vec{x}_i - \vec{x}_j, h_j) + f_i \frac{P_i}{\rho_i^2} \vec{\nabla}_i W(\vec{x}_i - \vec{x}_j, h_i) + \Pi_{ij} \vec{\nabla}_i \bar{W}_{ij} \right), \quad (3.16)$$

and

$$\frac{dA_i}{dt} = \frac{1}{2} \frac{\gamma - 1}{\rho_i^{\gamma-1}} \sum_j m_j \Pi_{ij} (\vec{v}_j - \vec{v}_i) \cdot \vec{\nabla}_i \bar{W}_{ij}, \quad (3.17)$$

where

$$\frac{4\pi}{3} h_i^3 \rho_i = N m_i \quad (3.18)$$

relates the choice for the number N of neighbors to the smoothing length h_i and therefore,

$$f_i \equiv \left(1 + \frac{h_i}{3\rho_i} \frac{\partial \rho_i}{\partial h_i} \right)^{-1} \quad (3.19)$$

are the coefficients f_i which fully include the correction terms for variable smoothing length. We also already added a term Π_{ij} which is the so-called *artificial viscosity*. This term is usually needed to capture shocks and its construction is similar to other hydrodynamical schemes. Usually, one adopts the form proposed by Monaghan and Gingold [66] and Balsara [67], which includes a bulk viscosity and a *von Neumann-Richtmeyer* viscosity term, supplemented by a limiter reducing angular momentum transport in the presence of shear flows at low particle numbers [68]. Modern schemes implement a form of the artificial viscosity as proposed by [69], based on an analogy with *Riemann* solutions of compressible gas dynamics. To reduce this artificial viscosity, at least in those parts of the flows where there are no shocks, one can follow the idea proposed by Morris and Monaghan [70]: every particle carries its own artificial viscosity, which eventually decays outside the regions which undergo shocks. A detailed study of the implications on the ICM of such an implementation can be found in [71]. There are various further improvements on the implementation a higher order artificial dissipation term [72, 73]. Even better suppression of

the artificial viscosity can be reached by following [72] in combination with higher order calculation schemes for velocity gradients (see [74]), as shown in [75].

Similarly, in the spirit of changing between following internal energy or entropy in the classical SPH formulations, one can change the principal, hydrodynamical variable from density ρ_i to the pressure P_i and obtain the so-called pressure formulation of SPH [76]. This can be further formulated in a much more generalized way, as shown in [77]. There, such a generalized formulation was obtained, starting from an x-weighted volume average

$$\bar{y} = y_i = \sum_j x_j W_{ij}(h_i), \quad (3.20)$$

the (x-weighted) volume element $\Delta\nu_i \equiv x_i/y_i$ and the generalized relation

$$P_i = (\gamma - 1)u_i \frac{m_i}{\Delta\nu_i} = A_i \left(\frac{m_i}{\Delta\nu_i} \right)^\gamma \quad (3.21)$$

between the pressure P_i , the internal energy per unit mass u_i and the entropy A_i . This leads to the set of generalized SPH equations

$$m_i \frac{d\vec{v}_i}{dt} = - \sum_j x_i x_j \left(f_{ij} \frac{P_j}{y_j^2} \vec{\nabla}_i W_{ij}(h_i) + f_{ji} \frac{P_i}{y_i^2} \vec{\nabla}_i W_{ij}(h_j) \right), \quad (3.22)$$

and

$$f_{ij} \equiv 1 - \frac{\tilde{x}_i}{x_j} \left(\frac{h_i}{3\tilde{y}_i} \frac{\partial y_i}{\partial h_i} \right) \left[1 + \frac{h_i}{3\tilde{y}_i} \frac{\partial \tilde{y}_i}{\partial h_i} \right]^{-1}. \quad (3.23)$$

For the choice of $x_i = \tilde{x}_i = m_i$, which implies $y_i = \tilde{y}_i = \bar{\rho}_i$ and $\Delta\nu_i = m_i/\rho_i$, and following the entropy A_i (e.g., $P_i = A_i \bar{\rho}_i^\gamma$), this set of equations will result in the entropy-conserving formulation of SPH as presented in [65]. For the choice of $x_i = \tilde{x}_i = (\gamma - 1)m_i u_i$, implying $y_i = \bar{P}_i$ and $\Delta\nu_i = (\gamma - 1)m_i u_i/P_i$, this results in a pressure–energy formulation. As now pressure is a kernel weighted quantity, contact discontinuities are properly treated. A third possibility is to choose $x_i = m_i A_i^{1/\gamma}$ which leads to a pressure–entropy formulation. For more details, see [77].

Considerable effort has also been made to involve Godunov methods into the SPH methods, but so far, they are still in the exploration phase, see [78–81].

3.2.5. Moving mesh (grid) methods

Substantial effort has gone into reformulating Eulerian methods as described in Section 3.2.2 into Lagrangian mesh approaches. More details on the idea of hydrodynamics on moving mesh for cosmological application can be found in the pioneering work by [82] and references therein. This early approach started from a regular mesh which then, by following the flow of the fluid, was deformed. The Euler equations were evolved by calculating the fluxes across the cell borders. An example of the

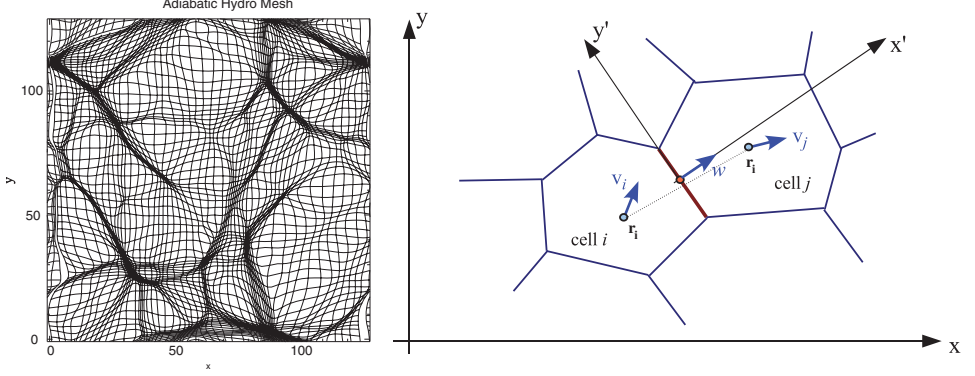


Fig. 3.4. Left panel: A layer through a cosmological, 128^3 moving mesh simulation. Figure taken from [82]. Right panel: Illustrating the concept of flux computation on a Voronoi mesh. Figure taken (and slightly adapted) from [83].

resulting mesh for a cosmological simulation can be seen in the left part of Fig. 3.4. One disadvantage (or challenge) of this technique in a practical application is that individual cells can be extensively deformed and stretched. Modern schemes circumvent this problem by constructing an unstructured mesh based on a Voronoi or Delaunay tessellation, see [84] and references therein. The relevant geometry of the cells, based on the mesh generating points $\vec{r}_i$ and $\vec{r}_j$ is illustrated in the right part of Fig. 3.4. The fluxes then have to be calculated at the centroid of the interface (note that this is not necessarily on the straight line between the two mesh generating points, as indicated by the dotted line)

$$\mathbf{Q}_i^{(n+1)} = \mathbf{Q}_i^{(n)} - \Delta t \sum_j A_{ij} \hat{\mathbf{F}}_{ij}^{(n+1/2)}. \quad (3.24)$$

The motion $\vec{w}$ of this interface is uniquely defined by the velocities $\vec{w}_i$ and $\vec{w}_j$, and the fluxes have to be calculated with the Riemann solver in the rotated frame (x', y') . A detailed description of this technique as well as its performance in test problems can be found in [84].

3.2.6. Meshless (particle) methods

Recently, a new class of Lagrangian methods, the so-called meshless formulations, were developed for astrophysical problems. More details can be found in [84, 85], which follow earlier, pioneering work by Vila and Coworker [86–88]. In short, its derivation starts from the integral form

$$\int [u(\vec{x}, t) \dot{\phi}(\vec{x}, t) + \vec{F}(u, \vec{x}, t) \cdot \nabla \phi(\vec{x}, t) + S(\vec{x}, t) \phi(\vec{x}, t)] d\vec{x} dt = 0 \quad (3.25)$$

of a scalar conservation law

$$\frac{\partial u}{\partial t} + \nabla \cdot (\vec{F} + \vec{a}u) = S, \quad (3.26)$$

where $u(\vec{x}, t)$ is a scalar field, $S(\vec{x}, t)$ is its source, $\vec{F}(u, \vec{x}, t)$ is its flux in a frame moving with velocity $\vec{a}(\vec{x}, t)$ and $\phi(\vec{x}, t)$ is an arbitrary differentiable function in space and time leading to the advective derivative $\dot{\phi}(\vec{x}, t) = \partial\phi(\vec{x}, t)/\partial t + \vec{a}(\vec{x}, t) \cdot \nabla\phi(\vec{x}, t)$.

Using a discretization through a set of particles i with a smoothing length $h(\vec{x})$ and a kernel function $W(\vec{x}, h)$, akin to what is done in SPH, the partitioning of the particles can be written as

$$\psi_i(\vec{x}) = w(\vec{x})W(\vec{x} - \vec{x}_i, h(\vec{x})), \quad (3.27)$$

where the number density of particles is $w(\vec{x})^{-1} = \sum_j W(\vec{x} - \vec{x}_j, h(\vec{x}))$, and the discretization of an arbitrary function $f(\vec{x})$ can be written as

$$\int f(\vec{x}) d\vec{x} \approx \sum_i f_i \int \psi_i(\vec{x}) d\vec{x} \equiv \sum_i f_i V_i, \quad (3.28)$$

where $V_i = \int \psi_i(\vec{x}) d\vec{x}$ is the effective volume of a particle i . Therefore, the discrete form of the integral equation (3.28) can be written as

$$\sum_i \int [V_i u_i \dot{\phi}_i + V_i F_i^\alpha (D^\alpha \varphi)_i + V_i S_i \phi_i] = 0. \quad (3.29)$$

Although in principal an SPH estimate for $(D^\alpha \phi)_i$ could be used, it is much better to use a more accurate meshless gradient estimate suggested in [87]. As shown in [84], this, together with integration of the first term by parts, permits the separation of $\phi(\vec{x}, t)$ and one obtains

$$\frac{d}{dt}(V_i u_i) + \sum_j [V_i F_i^\alpha \psi_j^\alpha(\vec{x}_i) - V_j F_j^\alpha \psi_i^\alpha(\vec{x}_j)] = V_i S_i. \quad (3.30)$$

This equation (and its extension to a general vector field $\vec{u}$) is very similar to the finite volume equation for the moving mesh method² but also somewhat similar to the SPH equations, except that the interactions between different particles is described in the source and flux terms, which can be obtained as the solution of an approximate Riemann problem between particles i and j . A closer inspection also reveals that only the projection on the direction between the particles is needed, e.g., the solution of the Riemann problem at the midpoint.³ This also means that the primitive variables have to be extrapolated to the midpoint, e.g., using linear extrapolation, and generally a flux limiter has to be applied, see discussion in

²Note that, however, Eq. (3.24) is in the integral form.

³More accurate would be the quadrature point at an equal fraction of the kernel length h_i and h_j , see discussion in [85] and references therein.

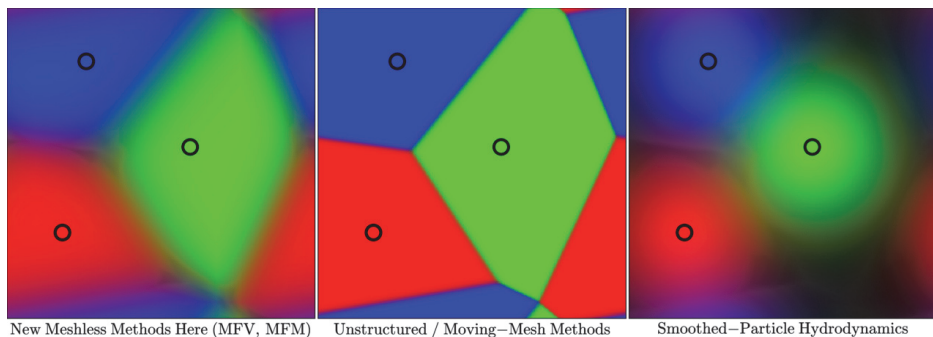


Fig. 3.5. Illustrating the conceptual differences in partitioning the volumes between meshless methods, unstructured grid and classical kernel weighted formalism, as used in SPH methods. Figure taken from [85].

[84, 85]. Figure 3.5 illustrates the differences in partitioning the volumes between mesh-less methods, unstructured (moving) grid and classical kernel weighted formalism (SPH).

3.3. Code comparison for cluster simulations

The Eulerian and Lagrangian approaches described in the previous sections should provide the same results when applied to the same problem. To verify that the code correctly solves the hydrodynamical set of equations, each code is usually tested against problems whose solution is known analytically. In practice, these are shock tubes or spherical collapse problems. Often, idealized hydrodynamical tests like the interaction of multi-phase fluids [90] reveal fundamental differences in different methods. Such differences can be driven by the formulation of the underlying fundamental equations (like no mixing in classical SPH) by the discretization (like the volume bias in SPH formulations) or the influence of numerical errors (like the departure of translation invariance in grid codes due to errors in the reconstruction).

In cosmology, a relevant test is to compare the results provided by the codes when they simulate the formation of cosmic structure, where finding an analytic solution is impractical; for example, [91] compares the thermodynamical properties of the IGM predicted by the *GADGET* (SPH-based) and *ENZO* (grid-based) codes. Another example of a comparison between grid-based and SPH-based codes can be found in [92].

A detailed comparison of hydrodynamical codes which simulate the formation and evolution of a galaxy cluster is therefore an extremely important test. A pioneering comparison was performed within the so-called Santa Barbara Cluster Comparison Project [93]. Here, 12 different groups, each using a code either based on the SPH technique (seven groups) or on the grid technique (five groups), performed a nonradiative simulation of a galaxy cluster from the same initial conditions. A more

recent comparison project, the so-called nIFTy galaxy cluster simulations [89], also involved modern SPH implementations as well as the moving mesh code *AREPO*. A similar agreement over large ranges was obtained for many of the gas properties in both studies, like the density, temperature and entropy profile as shown in Fig. 3.6). Both studies found significantly larger differences between mesh-based codes and classical particle-based codes to be present for the inner part of the profiles. However, as shown in [89] particle-based codes which include an explicit treatment of mixing produce results very similar to grid-based codes. It is worth mentioning that as soon as additional physics like star formation and AGN feedback is included, the discrepancies in the results obtained by the various numerical methods are no longer driven by such differences in the implementation of the underlying hydrodynamical treatment but the details contained in the realization of such additional processes [94].

3.4. Gas cooling

In cosmological applications, one is usually interested in structures with virial temperatures larger than 10^4K . In standard implementations of the cooling function $\Lambda(u, \rho)$, one assumes that the gas is optically thin and in ionization equilibrium. It is also usually assumed that three-body cooling processes are unimportant so as to restrict the treatment to two-body processes. For a plasma with primordial composition of H and He, these processes are collisional excitation of H^0 and He^+ , collisional ionization of H^0 , He^0 , and He^+ , standard recombination of H^+ , He^+ , and He^{++} , dielectric recombination of He^+ and free-free emission (bremsstrahlung). The collisional ionization and recombination rates depend only on temperature. Therefore, in the absence of ionizing background radiation, one can solve the resulting rate equation analytically. This leads to a cooling function $\Lambda(u)/\rho^2$ as illustrated in the left panel of Fig. 3.7. In the presence of ionizing background radiation, the rate equations can be solved iteratively. Note that for a typical cosmological radiation background (e.g., UV background from quasars, see [96]), the shape of the cooling function can be significantly altered, especially at low densities. For a more detailed discussion, see, for example, Chapter 6 and [3].

Additionally, the presence of metals will drastically increase the possible processes by which the gas can cool. As it becomes computationally very demanding to calculate the cooling function in this case, one usually resorts to a precomputed, tabulated cooling function. As an example, the right panel of Fig. 3.7, at temperatures above 10^5K , shows the tabulated cooling function from [97] for different metallicities of the gas, keeping the ratios of different metal species fixed to solar values. One further refinement is nowadays often done in simulations. Using the *Cloudy* code (ver. 96b4, [98]), the cooling and heating rates are often tabulated individually for a grid of UV intensities and for various different chemical elements. This allows the calculation of cooling rates self-consistently for arbitrary chemical compositions.

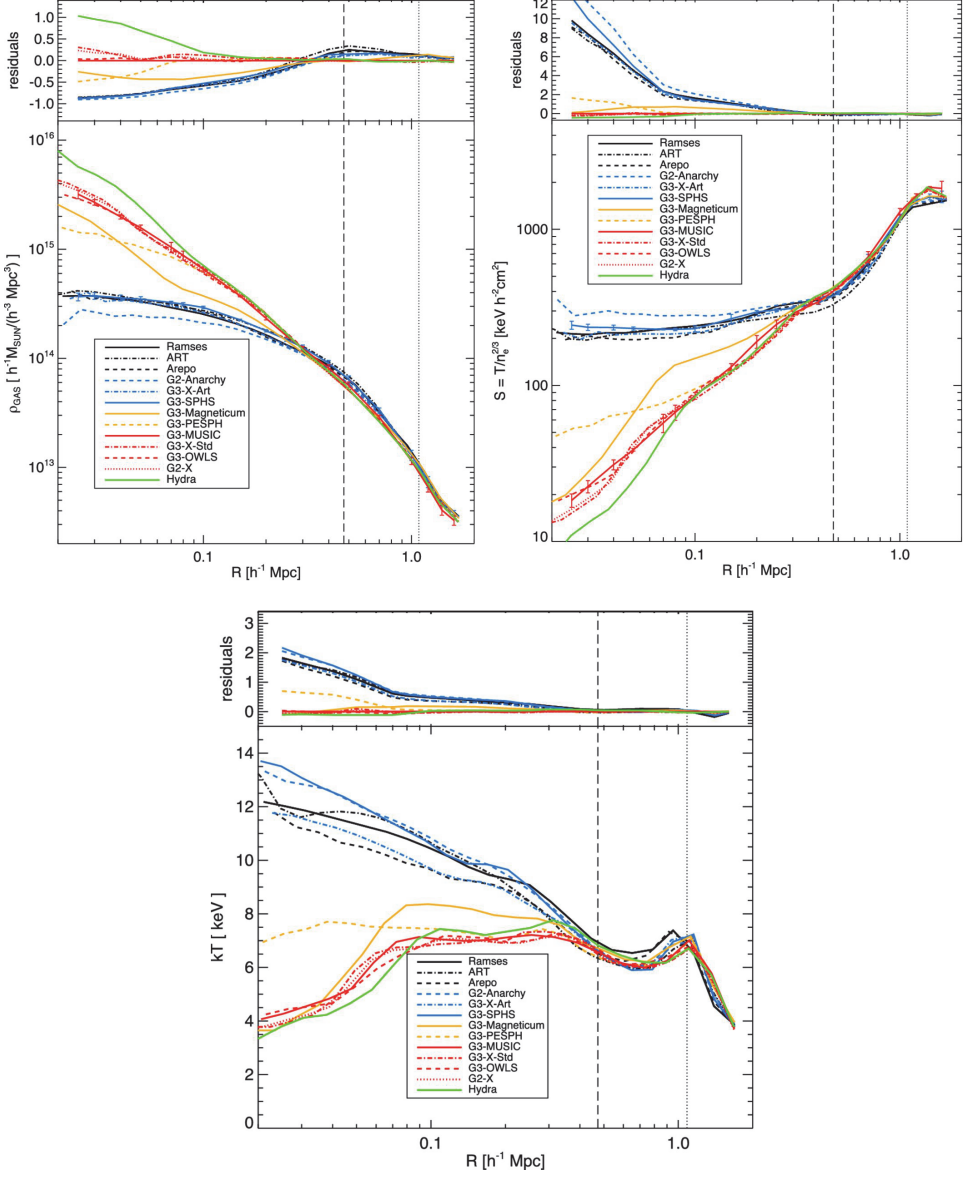


Fig. 3.6. One-dimensional density (upper left panel), temperature (lower panel) and entropy (upper right panel) of the simulated cluster at $z = 0$ of the nIFTy galaxy cluster simulations project [89]. The different lines show the result of the 13 different simulations. The main separation into two classes (classic SPH and grid or modern SPH methods) in the central part is clearly seen. Figure taken from [89].

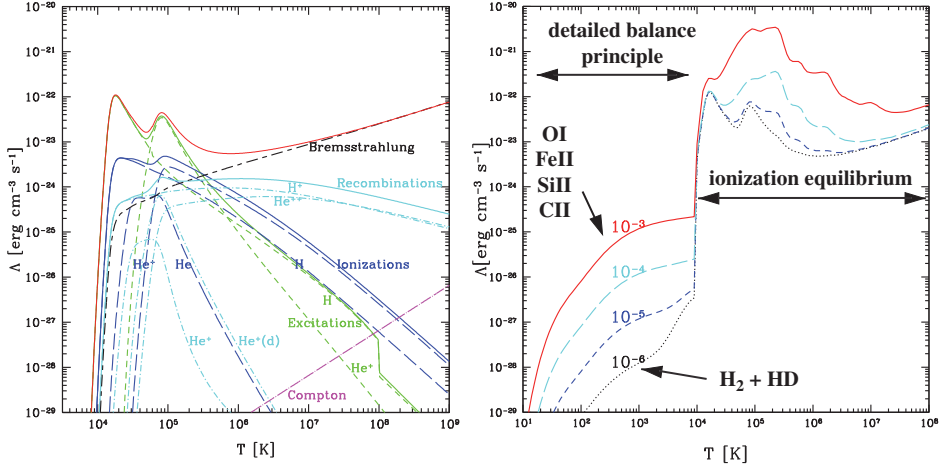


Fig. 3.7. Left panel: The total cooling curve (solid line) and its composition from different processes for a primordial mixture of H and He. Figure taken from [3]. Right panel: The total cooling curve as a function of different metallicity. The part below 10^4 K also takes into account cooling by molecules (e.g., HD and H_2) and metal lines. Figure taken from [95].

Note that almost all implementations solve the above rate equations (and therefore the cooling of the gas) as a “subtime step” problem, decoupled from the hydrodynamical treatment. In practice, this means that one assumes the density is fixed across the time step. Furthermore, the time step of the underlying hydrodynamical simulation is in general, for practical reasons, not controlled by or related to the cooling time scale. The resulting uncertainties introduced by these approximations have not yet been deeply explored and clearly leave room for future investigations.

For the formation of the first objects in halos with virial temperatures below 10^4 K, the assumption of ionization equilibrium no longer holds. In this case, one has to follow the nonequilibrium reactions, solving the balance equations for the individual levels of each species during the cosmological evolution. In the absence of metals, the main coolants are H_2 and H_2^+ molecules (see [99]). HD molecules can also play a significant role. When metals are present, many more reactions are available and some of these can contribute significantly to the cooling function below 10^4 K. This effect is clearly visible in the right panel of Fig. 3.7 for $T < 10^4$ K. For more details, see Chapter 6 and Refs. 100, 95 and references therein.

3.5. Star formation and feedback

Once radiative losses are taken into account, the drop out of cold gas into collisionless stars has to be modeled. This process is described in more detail in Chapter 6. In brief, when gas exceeds a certain density threshold, the resolution element (either the SPH smoothing length or the mesh size for *Eulerian* codes) is Jeans unstable and represents a convergent flow, it is assumed that the individual resolution element

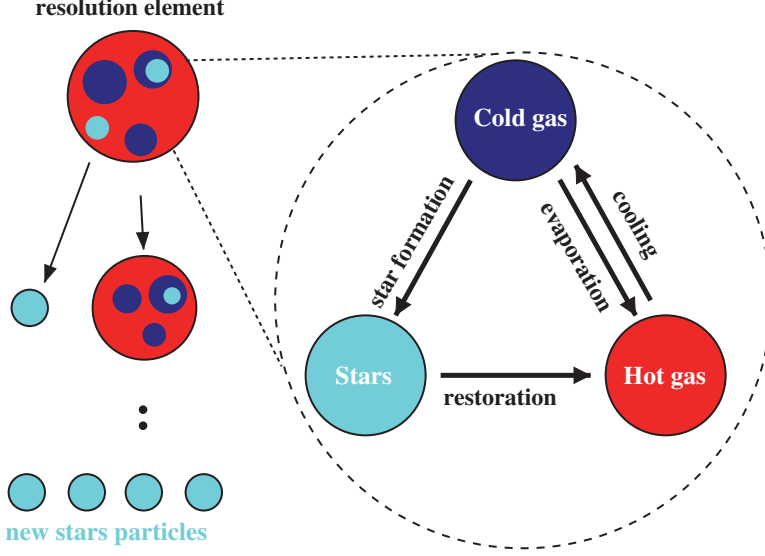


Fig. 3.8. Schematic sketch of the multi-phase subgrid model suggested by [101], indicating the different processes operating below the resolution scale.

becomes gravitationally unstable. In the simplest model [3], it is then assumed that it forms stars in a characteristic star formation time scale t_* . This characteristic time scale for star formation is usually taken to be the maximum of the dynamical and the local cooling time. For computational and numerical reasons, one waits until a significant fraction of the gas particle mass seems to have formed stars according to the rate above and then, a collisionless “star” particle is created from the parent star forming gas element whose mass is reduced accordingly, see left part of Fig. 3.8.

Improvements with respect to this model include an explicit subresolution description of the multi-phase nature of the interstellar medium which provides the reservoir of star formation. Such a subgrid model tries to model the global dynamical behavior of the interstellar medium by modeling the physical process driving the mass and energy flows between the different phases (e.g., cold, star forming clouds and stars are embedded in a hot medium), see right part of Fig. 3.8. This is typically done by calculating the equilibrium solution of the underlying set of differential equations [101]. An even more ambitious way would be to dynamically solve this set of differential equations as presented in [102], which typically even involves integration of the differential system on time scales below the typical, hydrodynamical time step.

3.6. Chemical enrichment

According to the above scheme of star formation, each star particle can be identified with a simple stellar population and characterized by a initial mass function

(IMF). Further, one usually assumes that all stars with masses larger than $8 M_{\odot}$ will end as type-II supernovae (SNII), which are believed to be the so-called core collapse supernovae (see [103] and references therein). Under this assumption, the total amount of energy (typically 10^{51} erg per supernova) that each star particle can release to the surrounding gas can be calculated. Within the approximation that the typical lifetime of massive stars which explode as SNII does not exceed the typical time step of the simulation, this is done in the so-called “instantaneous recycling approximation”, with the feedback energy deposited in the surrounding gas in the same step. Type-Ia supernovae (SNIa) are believed to arise from thermonuclear explosions of white dwarfs (see [104] and references therein). They lead to significantly delayed thermonuclear explosions (with respect to the time of creation of the star particle), as the white dwarf in the according binary system has to accrete matter from the companion and reach the mass threshold for the onset of thermonuclear burning and therefore cannot be included as easily in simulations. Stars in the asymptotic giant branch (AGB) contribute dominantly to the mass loss during the life of stars as well as to their nucleosynthesis of heavy elements (see [105] and references therein). Therefore, modern simulations have to follow the evolution of the stellar population in more detail to be able to calculate the chemo-energetic imprint from these most important contributors, SNIa, SNII, and AGB stars. This raises the need to integrate a set of complicated equations describing the evolution of a simple stellar population to be able to compute at each time the rate at which the current AGB stars pollute their environment by stellar winds and the rates SNIa and SNII are exploding at each time in order to properly treat their chemo-energetic imprint in the surrounding IGM and ICM. Here, we will only repeat a short, schematic description of such calculations. For a detailed review, see [106, 107] and references therein.

3.6.1. Initial mass function

The initial mass function (IMF) is one of the most important quantities in a model of chemical evolution. It directly determines the relative ratio between SNII and SNIa and therefore the relative abundance of α -elements and Fe-peak elements. The shape of the IMF also determines how many long-living stars will form with respect to massive short-living stars. In turn, this ratio affects the amount of energy released by supernovae and the present luminosity of galaxies which is dominated by low mass stars and the (metal) mass locking in the stellar phase.

The IMF $\phi(m)$ is defined as the number of stars of a given mass per unit logarithmic mass interval. A widely used form is

$$\phi(m) = dN/d\log m \propto m^{-x(m)}. \quad (3.31)$$

If the exponent x in the above expression does not depend on the mass m , the IMF is then described by a single power law. The most famous and widely used single power-law IMF is the Salpeter one (see [108]) that has $x = 1.35$.

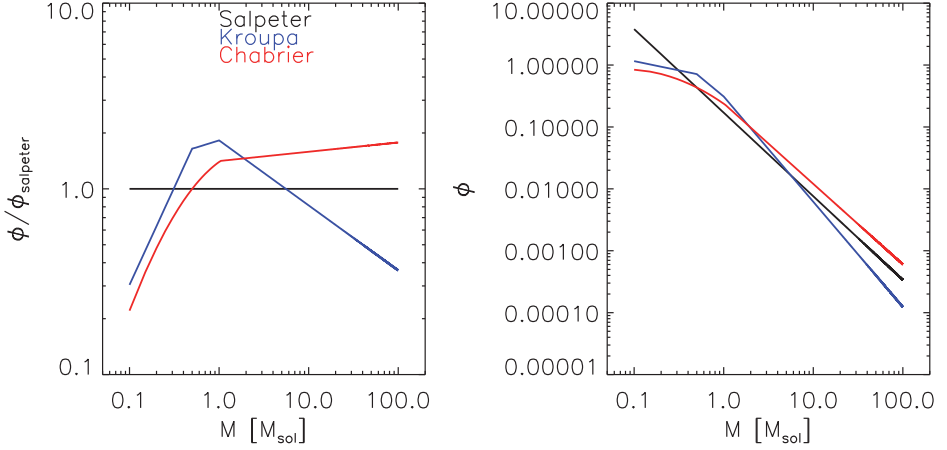


Fig. 3.9. Left panel: Kroupa and Chabrier IMF with respect to the classical Salpeter IMF. Right panel: Salpeter, Kroupa and Chabrier IMF.

More recently, different expressions of the IMF have been proposed in order to model a flattening in the low-mass regime that is currently favored by a number of observations. Kroupa ([109]) introduced a multi-slope IMF, which is defined as

$$\phi(m) \propto \begin{cases} m^{-1.3}, & m \geq 0.5 M_{\odot}, \\ m^{-0.3}, & 0.08 \leq m < 0.5 M_{\odot}, \\ m^{0.7}, & m \leq 0.08 M_{\odot}. \end{cases} \quad (3.32)$$

However, in many recent simulations (as well as in observational interpretation), the IMF proposed by Chabrier [110] is used, which has a continuous changing slope and is more top heavy

$$\phi(m) \propto \begin{cases} m^{-1.3}, & m > 1 M_{\odot}, \\ e^{\frac{-(\log(m) - \log(m_c))^2}{2\sigma^2}}}, & m \leq 1 M_{\odot}. \end{cases} \quad (3.33)$$

Figure 3.9 shows a comparison of the shapes of these different IMFs discussed above.

3.6.2. Lifetime functions

To follow such a simple stellar population, one needs to know the lifetime of the stars with different masses from stellar models, see Fig. 3.10. Different choices for the mass dependence of the lifetime function have been proposed in the literature. For instance, Padovani and Matteucci [111] proposed the expression

$$\tau(m) = \begin{cases} 10^{[(1.34 - \sqrt{1.79 - 0.22(7.76 - \log(m))})/0.11] - 9} & \text{for } m \leq 6.6 M_{\odot}, \\ 1.2 m^{-1.85} + 0.003 & \text{otherwise.} \end{cases} \quad (3.34)$$

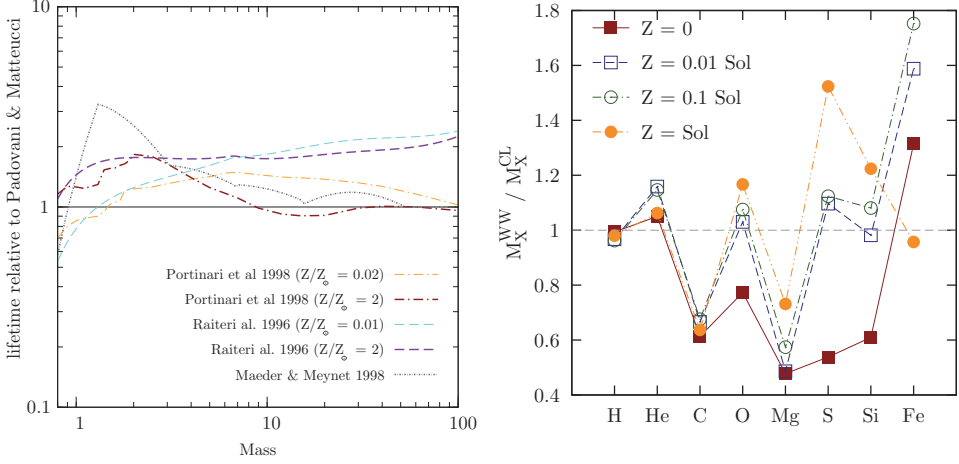


Fig. 3.10. Left panel: Ratio of lifetime functions from different stellar models. Figure taken from [107]. Right panel: Ratio of the predicted yields obtained from different stellar evolution model from [114] and [115]. Figure taken from [116].

An alternative expression has been proposed by Maeder and Meynet [112] and extrapolated by Chiappini *et al.* [113] to very high ($> 60 M_{\odot}$) and very low ($< 1.3 M_{\odot}$) masses:

$$\tau(m) = \begin{cases} 10^{-0.6545 \log m + 1} & m \leq 1.3 M_{\odot}, \\ 10^{-3.7 \log m + 1.351} & 1.3 < m \leq 3 M_{\odot}, \\ 10^{-2.51 \log m + 0.77} & 3 < m \leq 7 M_{\odot}, \\ 10^{-1.78 \log m + 0.17} & 7 < m \leq 15 M_{\odot}, \\ 10^{-0.86 \log m - 0.94} & 15 < m \leq 53 M_{\odot}, \\ 1.2 \times m^{-1.85} + 0.003 & \text{otherwise.} \end{cases} \quad (3.35)$$

The differences in such underlying lifetime functions will produce different evolutions and thereby different absolute, as well as relative, metal productions. Note also that so far, the lifetime functions are not assumed to depend on metallicity, although theoretically this might be expected.

3.6.3. Stellar yields

The ejected mass of the different metal species i produced by a star of mass m is called stellar yields $p_{Z_i}(m, Z)$. In models of stellar evolution, such yields also depend on the initial metallicity Z with which the star originally formed. As one stellar particle within the simulation typically represents a single stellar population, it is typically assumed that all stars formed with the same initial metallicity. Here, typically, the composition is ignored.

In general, one needs predictions for the three main processes: one for the continuous mass loss of AGB stars, one for SNII and one for SNIa. Up to today, such predictions still have significant uncertainties, mainly because of the still poorly understood mass loss through stellar winds in stellar evolution models, which depends on many additional physical process. This can be seen in the right panel of Fig. 3.10 which highlights such differences in the predicted yields by different stellar evolution models.

For mass losses through AGB stars, current simulations use tables predicted in [117] or [118]. For massive stars driving SNII, simulations use either [114], with some corrections, [119] or [120]. The most complete table for SNIa till date is presented in [121].

3.6.4. Modeling the enrichment process

Assuming a generic star formation history $\psi(t)$, we can now compute the rates for the different contributions.

3.6.4.1. Type Ia supernovae

As mentioned before, SNIa occurs in binary systems, having a mass range 0.8–8 $M_{\odot}$. Let m_B be the total mass of the binary system, and m_2 the mass of the secondary companion. We can now use $f(\mu)$ as the distributed binary systems with $\mu = m_2/m_B$ and define A (a typically value is 0.1) as the fraction of stars in binary systems that are progenitors of SNIa, both of which have to be given or obtained by a model. With these ingredients and the mass-dependent lifetime functions $\tau(m)$, we can model the rate of SNIa as

$$R_{\text{SNIa}}(t) = A \int_{M_{B,\text{inf}}}^{M_{B,\text{sup}}} \phi(m_B) \int_{\mu_{\text{m}}}^{\mu_{\text{M}}} f(\mu) \psi(t - \tau_{m_2}) d\mu dm_B, \quad (3.36)$$

where M_{Bm} and M_{BM} are the smallest and largest values allowed for the progenitor binary mass m_B . Then, the integral over m_B runs in the range between $M_{B,\text{inf}}$ and $M_{B,\text{sup}}$, which represent the minimum and the maximum values of the total mass of the binary system that is allowed to explode at time t . These values in general are functions of M_{Bm} , M_{BM} , and $m_2(t)$, which in turn depends on the star formation history $\Psi(t)$. In simulations, the stellar particles are in most typically modeled as an impulsive star formation event, and therefore $\psi(t)$ can be approximated with a Dirac δ -function.

3.6.4.2. Supernova type II and low- and intermediate-mass stars

Computing the rates of SNII, low-mass stars (LMS) and intermediate-mass stars (IMS) is conceptually simpler, since they are driven by the lifetime function $\tau(m)$ convolved with the star formation history $\psi(t)$ and multiplied by the IMF $\phi(m = \tau^{-1}(t))$. Again, since $\psi(t)$ is a delta function for our simple stellar population used

in simulations, the SNII, LMS, and IMS rates read

$$R_{\text{SNII|LMS|IMS}}(t) = \phi(m(t)) \times \left(-\frac{dm(t)}{dt} \right), \quad (3.37)$$

where $m(t)$ is the mass of the star that dies at time t . We note that the above expression must be multiplied by a factor of $(1 - A)$ for AGB rates if the interested mass $m(t)$ falls in the same range of masses which is relevant for the secondary stars of SNIa binary systems.

3.6.4.3. The equations of chemical enrichment

In order to compute the total metal release from the simple stellar population now, we have to fold the above rates with the yields for an element i from SNIa, SNII, and AGB stars $p_{Z_i}^{\text{SNIa|SNII|AGB}}(m, Z)$ for stars born with initial metallicity Z_i and compute the evolution of the mass $\rho_i(t)$ for each element i at each time t . As shown in [107], this reads

$$\begin{aligned} \dot{\rho}_i(t) = & -\psi(t)Z_i(t) + \int_{M_{BM}}^{M_U} \psi(t - \tau(m))p_{Z_i}^{\text{SNII}}(m, Z)\varphi(m) dm \\ & + A \int_{M_{Bm}}^{M_{BM}} \phi(m) \left[\int_{\mu_m}^{\mu_M} f(\mu)\psi(t - \tau_{m2})p_{Z_i}^{\text{SNIa}}(m, Z) d\mu \right] dm \\ & + (1 - A) \int_{M_{Bm}}^{M_{BM}} \psi(t - \tau(m))p_{Z_i}^{\text{AGB}}(m, Z)\varphi(m) dm \\ & + \int_{M_L}^{M_{Bm}} \psi(t - \tau(m))p_{Z_i}^{\text{AGB}}(m, Z)\varphi(m) dm. \end{aligned} \quad (3.38)$$

In the above equation, the first line describes the locking of metals in new born stars through the current, ongoing star formation $\psi(t)$ which in our case vanishes, as $\psi(t)$ is a delta function. M_L and M_U are the minimum and maximum masses of a star in the simple stellar population, respectively. Commonly adopted choices for these limiting masses are $M_L \simeq 0.1 M_\odot$ and $M_U \simeq 100 M_\odot$. For a comprehensive review of the analytic formalism, we refer to [122].

3.7. AGN feedback

In the current understanding, the feedback of AGNs operates in two different modes: the quasar mode during the main growth of the black hole, when large amounts of gas are flowing onto it and the radio mode at later time, when the black hole accretes at lower rate. In the latter one, powerful outflows in forms of jets are driven and believed to effectively shut down the cooling by heating the gas in the halo of massive galaxies.

There already exist a number of studies discussing galaxies and galaxy cluster simulations in cosmological context that also include black holes and the associated AGN feedback. Most of them follow the spirit of the black hole model implemented by Springel *et al.* [123] or are even based on it. Therefore, this model offers the ideal foundation to discuss the fundamental ideas behind the treatment of black holes in cosmological simulations.

In these models, black holes are typically described as sink particles which have fundamental properties like mass and accretion rate, which can be linked directly to their interaction with the ICM, like their energy input to the surrounding and observables like luminosity. The gas accretion onto a black hole of mass $M_\bullet$ is calculated according to the Bondi formula [124–126], multiplied by a so-called boost factor α ,

$$\dot{M}_B = \frac{4\pi\alpha G^2 M_\bullet^2 \langle \rho \rangle}{(\langle c_s \rangle^2 + \langle v \rangle^2)^{3/2}}, \quad (3.39)$$

where $\langle \rho \rangle$, $\langle v \rangle$, and $\langle c_s \rangle$ are mean values at the scale resolved by the hydrodynamical simulation, for example, computed using kernel weighted estimations in the case of SPH. The boost factor α was introduced to account for the limited resolution in simulations leading to smaller densities and larger temperatures near the black hole and typically is set to a value of 100. Several studies adapt the black hole model by using a boost factor which depends on the resolution [127, 128], density [129], pressure [130], or angular momentum [131]. High-resolution simulations of black hole accretion on sub-kpc scales [132] found that when including cooling and turbulence in their simulation, a boost factor of order of 100 is realistic, while for the adiabatic accretion, order of magnitude smaller boost factors are found. Hence, advanced models distinguish between hot and cold gas accretion and use the boost factors accordingly for the two components [133].

To estimate the AGN feedback,

$$\dot{E} = \epsilon_f \epsilon_r \dot{M}_\bullet c^2, \quad (3.40)$$

a constant value for the radiative efficiency ϵ_r is typically used [134] and ϵ_f is the efficiency with which the energy radiated from the black hole is coupled to the ISM [123]. Following [135], a steep transition of the feedback efficiency ϵ_f between radio-mode and quasar-mode, based on accretion rate of the BH, is then often used in current simulations (e.g., [21, 135, 136]). The energy is deposited either purely in the form of thermal energy, or, in some cases, used to inject bubbles (see also Fig. 3.11 and [135]) or kinetic energy [137] in the radio-mode to model the AGN feedback process in galaxy clusters more realistically [135].

However, this is only a rough approximation to the smooth transition which is observed (see, e.g., [140]) and also theoretically expected [142]. Furthermore, recent observations by Davis and Laor [138] and Chelouche [139] suggests that the radiative efficiency not only correlates with the accretion rate but also with the black hole

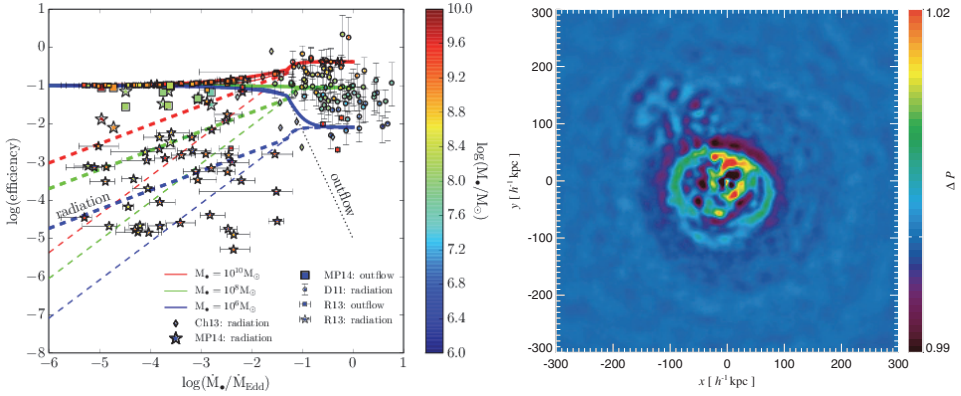


Fig. 3.11. Left panel: Collection of observational data points of the mechanical and radiative efficiencies taken from [138–141] overplotted with parameterized models. Figure taken from [133]. Right panel: Mass-weighted projected temperature and projected pressure maps of a $10^{15} M_{\odot}$ cluster simulated with AGN-driven cavities. Figure taken from [135].

mass. Therefore, modern simulations [133] include such observed dependencies of the efficiency parameters in the form of parameterized models, see Fig. 3.11.

3.8. Current state

Most current large-scale high-resolution cosmological simulations are based on pure gravitational physics. These simulations are usually complemented by running the so-called semianalytic models (SAMs) of galaxy formation. While SAMs provide a realistic description of the properties of galaxy populations, they provide at best indirect information on the properties of the IGM and do not properly include the dynamical effects of the baryons on structure formation, which is highly relevant for the study of environmental effects.

Attempts have been pursued to perform large-scale, high-resolution hydrodynamical simulations of galaxy formation like Illustris⁴ [26] or EAGLE⁵ [27], but these high-resolution simulation still covers very small volumes in cosmological context (e.g., $< 100 \text{ Mpc}$).

To bridge the scales between galaxy formation simulations and large cosmological volumes, simulation campaigns like the *Magneticum Pathfinder*⁶ project have to combine different simulations with different box sizes and cosmological volumes, simulated with the same physical processes taken into account. Figure 3.12 shows a visualization of the different boxes from the pathfinder project. The combination of the different boxes allows one to study the formation of objects covering almost

⁴www.illustris-project.org.

⁵icc.dur.ac.uk/Eagle.

⁶www.magneticum.org.

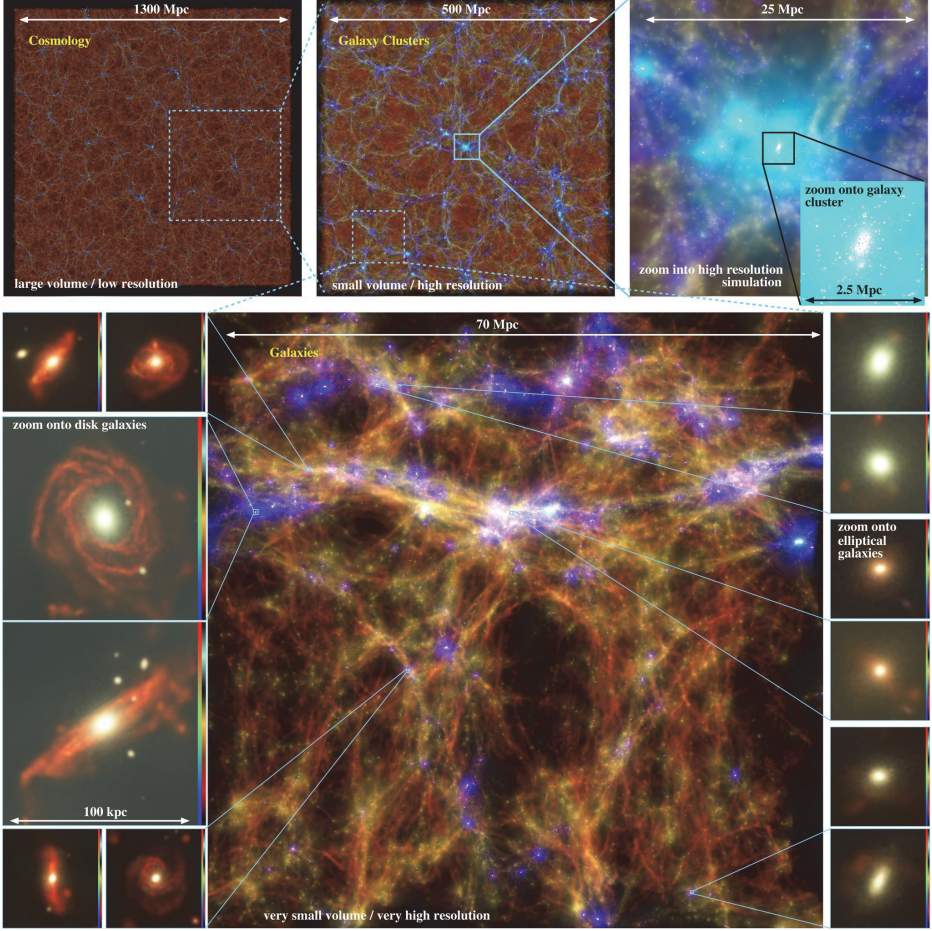


Fig. 3.12. Visualization of the different boxes of *Magneticum Pathfinder* as overview. Zooming from the largest scales (Gpc scales) into galaxy clusters (Mpc scales) and even further down onto individual galaxies (tens of kpc scales).

four orders of magnitudes in mass, even when considering only well-resolved objects with more than 10^4 particles. Figure 3.13 shows the evolution of the mass function obtained from these hydrodynamical simulations, together with the best fitting halo mass function and compared to the dark matter control simulations. Although small, it is important to understand the imprint of the baryonic physics in the halo mass function, as these effects will be essential for the cosmological interpretation of future surveys like eROSITA [28]. The growing computational power of current and future HPC facilities, together with the improvements in numerical methods, will allow us to study the formation process of cosmological structures in so far unrivaled detail and to better link the small-scale physical processes of galaxy formation to the formation of the large-scale structures.

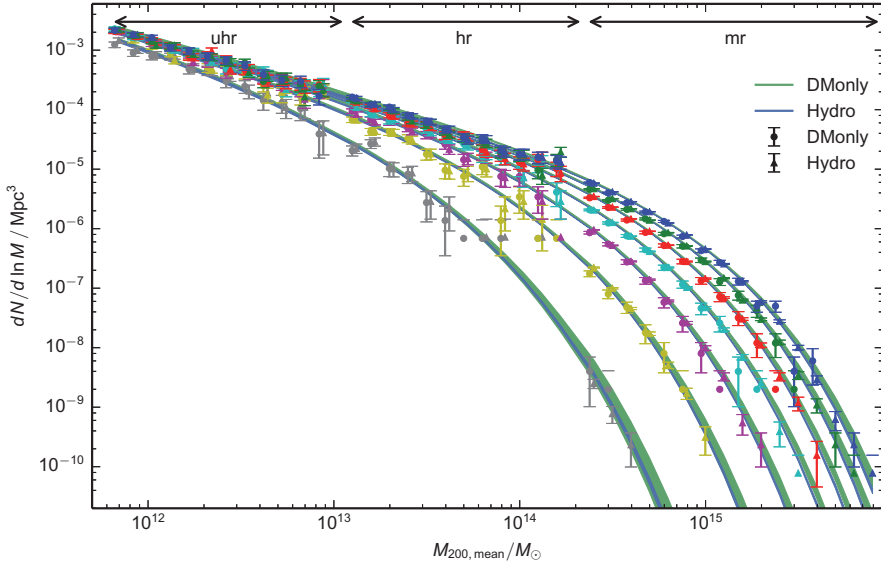


Fig. 3.13. Halo mass function $dN/d \ln M$ from the *Magneticum Pathfinder* simulations. Redshift is increasing from top to bottom and takes values $z = 0, 0.13, 0.3, 0.5, 0.8, 1.2, 2$. The data points are slightly offset in mass for improved readability. Figure taken from [28].

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Chapter 4

First Stars in Cosmos

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First stars are the very first light of the Universe after the recombination. They illuminate, ionize, and heat up the surrounding material by the radiation. They also explode to put kinetic energy into the interstellar medium, thereby spreading the elements heavier than helium, such as carbon, oxygen, iron, etc., which are indispensable for the birth of lives. The formation process of these stars has been studied intensively to predict that the significant fraction of these stars is rather massive, $\sim 10\text{--}10^3 M_\odot$, although still little evidence has been found observationally. In this chapter, the theoretical challenges and results in the last two decades on this issue, as well as the key observations which constrain the theory are described. In addition, future prospects in the field are discussed.

4.1. Introduction

4.1.1. *First stars trigger the evolution of the universe*

The history of the *Cosmos* has started with the *Big Bang*. The elements synthesized at the beginning were hydrogen, helium, and a trace amount of lithium and beryllium. The present universe essentially consists of these elements, but thanks to the nuclear fusion in stars, 2% of baryons are turned into heavier elements such as carbon, oxygen, iron, etc.

The definition of the *first stars* are not so clear, but they are normally regarded as the stars born in the primitive sites of the universe unperturbed by the stars/galaxies that had formed prior to them. Similar terminology “Population III (Pop III)” is also often used, but they are considered to be the metal-free stars that involve the former definition.

In any case, these stars are born to form elements heavier than helium for the first time in the history of the universe. As we will see later, majority of these stars are considered to be very massive $\sim 10\text{--}10^3 M_\odot$, and a significant fraction of them

ends up as supernova explosions. As a result, the elements heavier than helium — frequently called as “metals” — diffuse into the interstellar gas, which will collapse by gravity to form new generation of stars, planets, and lives.

The first stars are not only the prototype of the factory of element generation but also light up the dark universe by the nuclear fusion energy, ionize, and heat up the surrounding materials, and spark the cosmic reionization. The explosion at the death of these stars inject directly huge kinetic energy into the interstellar medium that accelerate, compress, and heat up the surrounding gas to turn it into the seed of next generation of stars.

In this manner, the birth of the first stars is the beginning of the thermal evolution of the universe and life cycle of stars/galaxies and thus the lives of ourselves.

4.1.2. *A brief historical review*

In this section, we briefly summarize the history of the studies on the formation of first stars. It has a rather long history — that seems to have the embryo in 1960s. In Ref. 1, the gravitational collapse of a primordial gas cloud is discussed, using simplified one zone model, following the studies on local star formation. After this ice break, studies of the thermal evolution of collapsing primordial clouds were released, adding missing and important physics [2–8]. According to these studies, it was already known by the end of the 1980s that the main coolant of the primordial gas is H_2 molecule and its inefficient cooling causes a rather high temperature of collapsing gas. However, these studies could not be considered a sweeping trend. There are a few reasons for this — the standard cosmological model, i.e., the Cold Dark Matter (CDM) paradigm was not established until the late 1980s, the computational resource was far from sufficient, and zero-metallicity stars, i.e., Pop III stars, had not been discovered probably because of their rareness.

However, in the late 1980s, the CDM paradigm was established to provide proper initial conditions of the galaxy formation as well as the first star formation. Combined with the development of numerical resources/methodology, the first star formation has become a well-defined and compassable problem for theoretical astrophysicists. Most of the attention of theoretical researchers were directed to the formation of galaxies initially because their distribution, morphology, luminosity, etc., could be compared with the observations. However, as the complexity of the galaxy formation processes, which always require various subgrid physics, had been revealed, the importance of the study of star formation in the forming galaxies, especially the first star formation, was recognized.

Against this background, from late 1990s to early 2000s, the numerical simulations of first star formation from cosmological initial conditions were performed intensively to reveal the nature of these stars [9–14]. It is worthwhile to note that the explosive progress of these studies were allowed by the development of zoom-in techniques such as Adaptive Mesh Refinement (AMR) or Particle Splitting. Parallel to this trend, one-dimensional but detailed chemistry/radiation hydrodynamic

calculations [15] were also carried out to understand how the proto-first-stars form and evolve. Thanks to these efforts, until mid-2000s, the birth of proto-first-stars in Λ CDM universe had been understood pretty well.

However, the proto-first-stars are just tiny embryos born at the end of the runaway collapse phase of star formation. They accrete much larger amount of mass after their birth in the mass accretion phase. It is possible to assess the mass accretion rates onto the proto-first-stars by the density/velocity distributions of surrounding gas at their birth with an assumption of spherical accretion. The expected mass accretion rate is very high $\sim 10^{-3}$ – $10^{-2}M_{\odot}$, which is roughly 100–1000 times larger than the present-day counterparts. Hence, the final mass of the first stars were thought to be very massive, nominally in the range of $\sim 10^2$ – $10^3M_{\odot}$ [14].

Therefore, as a first approximation, these stars are very massive. However, in reality, the accreting gas has angular momentum, which forces them to form accretion disks. Furthermore, the evolving protostar emits ultraviolet radiation to suppress the accretion. All these effects have to be addressed to obtain the final mass of the first stars. Direct simulations are desirable, but it is not possible to follow the evolution after the birth of the proto-first-stars by ordinary methodology used in the runaway collapse phase, since the time scale around the proto-first-star is too short to follow the whole dynamical evolution of the accreting gas onto the proto-first-star.

In 2000s, studies on the mass-accretion phase had begun. Initially, spherically symmetric model of proto-stellar evolution was employed to investigate the radiative feedback from the proto-first-star [16–18]. They found that the mass accretion could be suppressed by the ultraviolet radiation, but still uncertain because of the assumption of steadiness.

In 2010s, dynamical multi-dimensional numerical models without radiative feedback came out, revealing that the accretion disk forms around the proto-first-star. The disks are gravitationally unstable and fragment into many secondary stars [19–26]. The fate of these secondaries are still in debate until now, but in any case, some are falling onto the primary star to merge and some survive in a multiple system or get ejected to unbound state. The mass of these secondaries could be $\ll 1M_{\odot}$ if they escape from central dense region of the host cloud. Multi-dimensional dynamical models with radiative feedback also became available [27–34]. In these simulations, radiative feedback are found to be very efficient, and it suppresses the mass accretion in many cases. At the same time, a new branch along which the feedback becomes inefficient was found, where the intrinsic mass accretion rate is very high $> 10^{-2}M_{\odot}$. In such cases, the mass accretion does not stop until the falling gas is exhausted — the star can grow up to $\sim 10^3M_{\odot}$. In most rare cases in which very rapid accretion rate is achieved, it can grow even more massive than $10^4M_{\odot}$, which will end up as a direct collapse black hole to be the seeds of supermassive black holes [35]. Consequently, the mass distribution of the first stars is considered to spread from $\sim 1M_{\odot}$ to $\sim 10^3M_{\odot}$ (and can grow to $\sim 10^5M_{\odot}$ in the rarest cases).

From an observational point of view, direct detection of the first stars is impossible even with the next generation facilities such as JWST or TMT. Hence, it is logical that we should try to find the trace of the first stars from various channels. Most simple-minded observation is to search the stars with no metal absorption lines, which has been carried out from the last century, but in vain. Most common strategy is to observe the abundance ratio in the low metallicity systems such as metal-poor stars in the near field or damped Lyman- α (DLA) systems. If these metal-poor systems are the remnant of the first stars, their abundance ratio reflects that of the progenitors. It has been confirmed that the averaged abundance ratio of extremely metal-poor stars ($[\text{Fe}/\text{H}] < -3$) and that of the DLAs are consistent with that of the ejecta of core collapse supernova of several tens of solar masses [31, 36, 37]. On the other hand, almost no indication has been found that they came from the pair instability supernova (PISN) which is more massive than the core collapse supernova, despite the theoretical prediction that they are common among first stars.

As seen above, from the theoretical side, first star formation is understood to some extent based on the framework of Λ CDM cosmology, but we still do not know the final mass distribution of these stars. Furthermore, we still do not have enough information from observations to constrain the theoretical models. In this chapter, we summarize the state-of-art knowledge on the first star formation to contribute further research on this issue.

In the following sections, physical processes of first star formation is described in chronological order. Then we describe the comparison of the theory with observations. Finally, we discuss the future prospects.

4.2. Formation of Host Minihalos

In Λ CDM cosmology, small-scale density perturbations grow and collapse faster than the perturbations in larger scales because of the initial spectrum. The minihalos of 10^5 – $10^6 M_\odot$ form at $z \sim 30$ – 20 from $2 - 3\sigma$ density fluctuations and eventually host first stars via radiative cooling by H_2 molecules. In this section, we describe how these minihalos form and host first stars.

4.2.1. Growth of density perturbations

In the linear regime, the density perturbation $\delta(M)$ filtered over a mass scale M is proportional to the scale factor in Einstein–de Sitter universe. Therefore, the linear density fluctuation at a given redshift is

$$\delta_{\text{linear}}(M, z) \simeq \delta_{\text{linear}}(M, 0)/(1+z), \quad (4.1)$$

where $\delta_{\text{linear}}(M, 0)$ denotes the linearly extrapolated density fluctuation at $z = 0$. On the other hand, the dense region collapses to form a virialized halo when the linearly

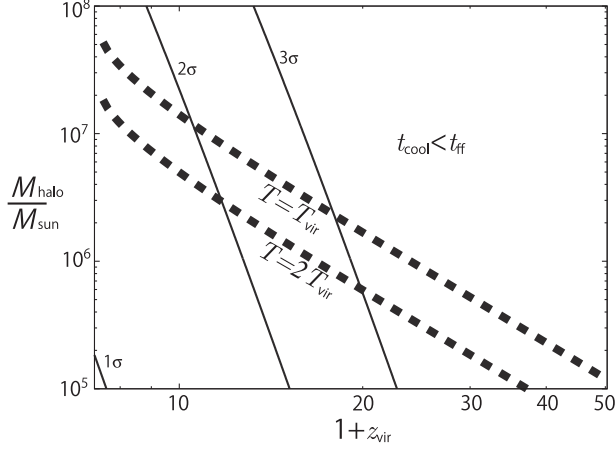


Fig. 4.1. Minimal cooling mass of minihalos. Thick dashed: The locus along which $t_{\text{cool}} = t_{\text{ff}}$ is satisfied in the minihalo with a given collapse redshift (z_{vir}) and a temperature (T). Two lines correspond to the cases of $T = T_{\text{vir}}$ and $2T_{\text{vir}}$ considering the scatter of the temperature in the virialized minihalo. Thin solid: the collapse redshift–halo mass relation with given amplitudes of 1–3 σ density fluctuations in Planck cosmology.

extrapolated density fluctuation $\delta_{\text{linear}}(M, z)$ equals 1.69. Hence, the redshift when the dense region turns into a virialized object (z_{vir}) is given as

$$z_{\text{vir}} = \delta_{\text{linear}}(M, 0)/1.69 - 1. \quad (4.2)$$

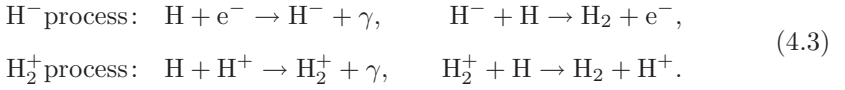
For Λ CDM cosmology, the growth rate of the density perturbations and the threshold value 1.69 differ from those in this case, but the differences are small for high redshift such as $z > 20$ [38]. The averaged fluctuation $\sigma_0(M) = \sqrt{\langle \delta_{\text{linear}}^2(M, 0) \rangle}$ is well determined by the CMB observations by Planck [39] and the cosmological model [40]. In Fig. 4.1, the collapse redshifts (i.e., the formation redshift) vs. the halo masses are plotted by the solid lines for 1 σ_0 , 2 σ_0 , and 3 σ_0 density perturbations. In this way, we obtain the formation epoch of the halo with a given mass and an overdensity. However, it does not directly mean that they become the site of first star formation. We have to consider whether these halos can host first stars, since those have to cool to form dense gas cloud to trigger the star formation. In the next section, we consider the cooling condition of the gas in the halos, with special attention to for the nature of primordial gas.

4.2.2. Primordial chemistry and H_2 cooling

The primordial gas contains hydrogen and helium, but do not have heavier elements as well as the dust grains which exist in the interstellar gas in the nearby universe. The cooling process related to H and He are bound–bound transition of electrons, ionization, recombination (free–bound transition), bremsstrahlung (free–free transition), and Compton cooling. These processes are fairly efficient for $T > 10^4$ K, but

almost no emission rate below 10^4 K, because these processes are activated under the condition that a significant fraction of atoms is ionized or the quantum states of electrons are excited. For instance, the energy gap of a hydrogen atom between the bound state and the first excited state is 10.2 eV, which corresponds to $\sim 10^5$ K. In primordial gas at 10^4 K, the atoms/electrons in the tail of Maxwell–Boltzmann distribution can marginally excite this transition via collision. Hence, we have a steep break at $\sim 10^4$ K in the cooling function of primordial gas.

Therefore, the primordial gas composed of atomic hydrogen and helium does not cool below 10^4 K, which gives the lower bound of the virial temperature of halos that cool and collapse to form dense gas clouds. However, if we consider the nonequilibrium state in the collapsing gas clouds, H and He are not the only compositions, but small amounts of H_2 form via the following two paths:



So, electrons and protons catalyze the formation of H_2 . H_2 molecules have much lower energy transition levels — the rotational–vibrational levels — than that of H/He atoms. The ratio among the typical energy gaps of the electron transition (E_{el}), vibrational transition (E_{vib}) and rotational transition (E_{rot}) is given as [41]

$$E_{\text{el}} : E_{\text{vib}} : E_{\text{rot}} \sim 1 : \left(\frac{m_{\text{e}}}{m_{\text{p}}} \right)^{1/2} : \left(\frac{m_{\text{e}}}{m_{\text{p}}} \right), \quad (4.4)$$

where m_{e} and m_{p} represent the mass of electrons and protons, respectively. Since the mass ratio of these two is ~ 1800 , the rotational–vibrational energy is much lesser than the energy of electron transitions. In fact, the lowest rotational energy gap of H_2 molecules is 0.0147 eV, which is much lesser than 10.2 eV, the gap of the Lyman- α .

This lowest rotational energy gap is a forbidden transition since H_2 is a homonuclear diatomic molecule. The energy of the lowest allowed transition is 0.044 eV which corresponds to 512 K. Hence, the gas can cool as low as ~ 100 K in the presence of enough amount of H_2 molecules, considering the tail of Maxwell–Boltzmann velocity distribution. In this manner, the halo whose virial temperature is less than 10^4 K is able to cool via H_2 cooling.

4.2.3. Cooling of the gas in minihalos

In the Λ CDM universe, less massive halos collapse earlier, followed by the merging of these small halos to form more massive ones. Therefore, first stars are expected to form in the smallest halos in which the baryonic gas can cool to form dense clouds. The smallest halo mass that can cool by radiative cooling can be obtained if we assess the amount of H_2 in the collapsing primordial gas. Simple one-zone modeling

enables us to estimate H_2 fraction in such clouds [42–44], as well as one-dimensional collapse simulation [45].

Here, we describe the time-scale arguments on the cooling condition of the minihalos. Following the Rees–Ostriker arguments [46] of galaxy formation, the cooling condition can be written as

$$t_{\text{cool}} < t_{\text{ff}}, \quad (4.5)$$

where

$$t_{\text{cool}} \equiv \frac{1}{\gamma - 1} \frac{k_{\text{B}} T}{n_{\text{H}} y_{\text{H}_2} \Lambda_{\text{H}_2}}, \quad (4.6)$$

$$t_{\text{ff}} \equiv \sqrt{\frac{3\pi}{32G\rho}}. \quad (4.7)$$

Here, t_{cool} is the cooling time and t_{ff} is the free-fall time. n_{H} denotes the number density of the hydrogen nuclei, y_{H_2} is the number density of H_2 molecules normalized by n_{H} , ρ and T are the mass density and the temperature of the gas in the minihalo, respectively. Λ_{H_2} is the radiative cooling rate via H_2 rotational–vibrational transitions, which is given by an empirical formula in the low-density limit [47] ($n_{\text{H}} \ll 10^4 \text{cm}^{-3}$) as

$$\begin{aligned} \Lambda_{\text{H}_2}(n_{\text{H}} \rightarrow 0) \\ = 10^{(-103 + 97.59 \log_{10} T - 48.05 (\log_{10} T)^2 + 10.8 (\log_{10} T)^3 - 0.9032 (\log_{10} T)^4)} [\text{erg cm}^3 \text{s}^{-1}]. \end{aligned} \quad (4.8)$$

Using the above relations, we obtain minimally required y_{H_2} for the minihalo to cool as follows:

$$y_{\text{H}_2} > \frac{1}{\gamma - 1} \frac{k_{\text{B}} T}{n_{\text{H}} \Lambda_{\text{H}_2} t_{\text{ff}}}. \quad (4.9)$$

The initial fraction of H_2 in the uniformly expanding universe is $y_{\text{H}_2} \sim 10^{-6}$ [47], which is too low for the gas to cool at $T_{\text{vir}} < 10^4 \text{K}$ [48]. Then, we need to assess y_{H_2} in the collapsing minihalo where H_2 form via nonequilibrium reactions. H_2 molecules mainly form through the H^- process described in (4.3), which is limited by the first reaction. Hence, the formation rate of H_2 is given by the reaction rate of the first reaction,

$$\frac{dy_{\text{H}_2}}{dt} \simeq k_{\text{f}} n_{\text{H}} n_{\text{e}}, \quad (4.10)$$

where k_{f} denotes the rate of the first reaction in (4.3), given as [47]

$$k_{\text{f}}(T) = 1.4 \times 10^{-18} T^{0.928} \exp(-T/16200) [\text{cm}^3 \text{s}^{-1}]. \quad (4.11)$$

The next step is to estimate the duration of H_2 formation. It should be the free-fall time t_{ff} , however, the electron number density on the right-hand side of Eq. (4.10)

could decrease during the collapse. If the recombination time scale is shorter than the free-fall time, the catalyst of the reaction disappears, which means the formation of H_2 ceases within the recombination time. Comparing the recombination time with the free-fall time in the virialized minihalos, the former is longer than the latter if

$$\frac{1}{k_{\text{rec}}(T)n_e} > t_{\text{ff}}, \quad (4.12)$$

where $k_{\text{rec}}(T)$ is the recombination rate which is given as

$$k_{\text{rec}}(T) = 2.06 \times 10^{-11} T^{-1/2} (5.77 - 0.567 \ln T + 0.00862 (\ln T)^2) [\text{cm}^3 \text{s}^{-1}]. \quad (4.13)$$

This function is obtained by fitting of the table in Ref. 49. Substituting T in Eq. (4.12) with the virial temperature T_{vir} of a minihalo with a given collapse redshift z_{vir} and mass M_{minihalo} , and replacing the electron fraction y_e by 3×10^{-4} [47], the residual value in the uniform background, we have

$$M_{\text{minihalo}} \gtrsim 1200 M_{\odot} \left(\frac{1 + z_{\text{vir}}}{100} \right). \quad (4.14)$$

Hence, under the above condition, we can use t_{ff} as the duration while H_2 formation proceeds. As a result, y_{H_2} is given as follows:

$$y_{\text{H}_2} \simeq \frac{dy_{\text{H}_2}}{dt} t_{\text{ff}} = k_{\text{f}} n_{\text{H}}^2 y_e t_{\text{ff}}. \quad (4.15)$$

The electron fraction y_e is replaced again by 3×10^{-4} , which is the value of the uniform background.

Combining Eqs. (4.9) and (4.15), we have

$$\frac{k_{\text{B}} T}{k_{\text{f}}(T) \Lambda_{\text{H}_2}} > (\gamma - 1) n_{\text{H}}^2 t_{\text{ff}}^2 y_e. \quad (4.16)$$

Thus, we obtain the cooling condition on the gas temperature for a minihalo to cool.

Figure 4.1 shows the cooling condition for the minihalos of various mass and formation time. Thick dashed curves denote the cooling condition, above which the minihalo cools via H_2 transitions. Two curves correspond to the cases substituting the virial temperature T_{vir} or $2T_{\text{vir}}$ into the gas temperature T in Eq. (4.16), considering the scatter of the temperature in the minihalos. Three thin curves correspond to the collapse redshift of halos of 1σ , 2σ and 3σ density perturbations. If we regard $> 3\sigma$ density perturbations as the earliest collapsing region with a given scale, the minimum mass of the cooling halo is $\sim 10^6 M_{\odot}$ which forms at $z \gtrsim 20$. Those are called as “minihalos”, and they are the hosts of first stars.

Cosmological simulations also confirm these results [14]. The left panel of Fig. 4.2 shows gas density distribution of a slice at $z = 17$. Filamentary structures are found as in the large-scale structure simulations, and dense clumps form at the nodes of the filaments. These are located at the center of minihalos, and as massive

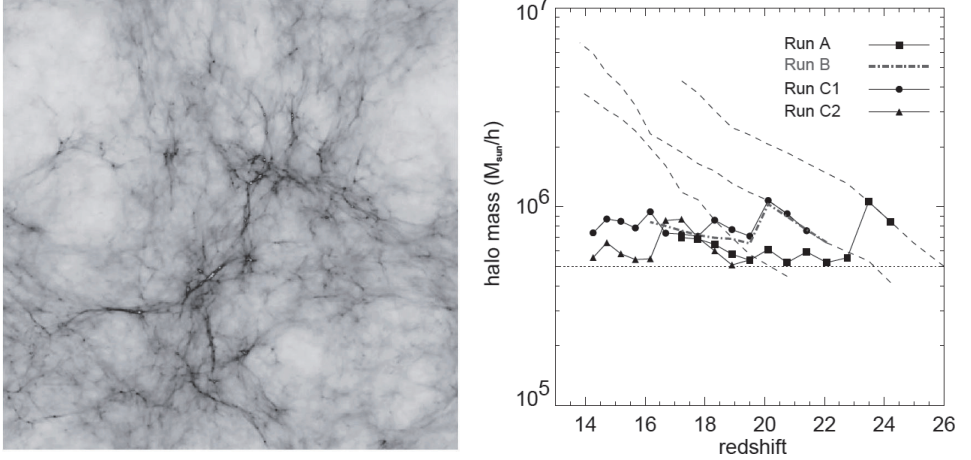


Fig. 4.2. Left panel: Projected gas density distribution of cosmological volume $(600h^{-1}\text{kpc})^3$ box at $z = 17$. Right panel: Minimal mass of minihalos that host cold dense gas clumps in various runs [13].

as $100\text{--}1000 M_{\odot}$ when they reach $n_{\text{H}} \sim 10^4 \text{cm}^{-3}$. This mass scale is comparable to the Jeans mass of these clouds. The right panel describes the minimum mass of the halos found in the cosmological simulations. The minimum mass falls onto several times $10^5 M_{\odot}$ in these simulations, which is roughly consistent with the analytic arguments discussed above, although they explicitly take into account the effects of gas heating by merging with the small structures. In the next section, we will discuss the thermal evolution of these primordial gas clumps during further collapse to form proto-first-stars.

4.3. Runaway collapse of the cooled gas

The cold gas clumps formed in the minihalos proceed to further gravitational collapse by cooling with various physical processes. Here, we describe the thermal processes in the collapsing primordial gas. The left panel of Fig. 4.3 shows the evolution of gas temperature at the center of the core as functions of density, while the fractions of H_2 molecules are plotted in the right panel. We utilize the one-zone approximation to assess physical quantities in the collapsing core [50, 51], which is in good agreement with the results of cosmological three-dimensional calculations [14]. The solid curve denotes the evolution of primordial gas cloud. The labels denote the phases of the evolution following Ref. 14.

Overall evolution of the temperature for $n_{\text{H}} > 10^4 \text{cm}^{-3}$ is gradual, which can be approximated by a single power of a polytrope with $\Gamma = 1.09$ [15]. It is known that the collapse of such a cloud by self-gravity proceeds in a runaway fashion and converges to a self-similar solution [52–54].

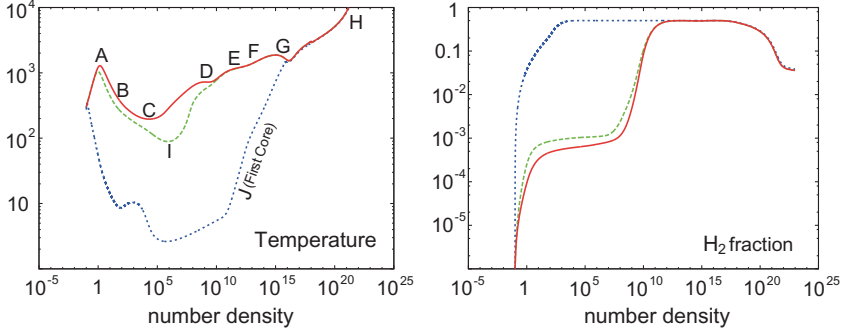


Fig. 4.3. Thermal evolution of the collapsing gas clouds are shown. Left panel: gas temperature as functions of gas number density of the collapsing core. Right panel: evolution of the fraction of H_2 . Solid curve: primordial, dashed: primordial with ionization by cosmic rays/radioactive elements, dotted: interstellar gas. The labels in the left panel basically follow the notation in Ref. 14.

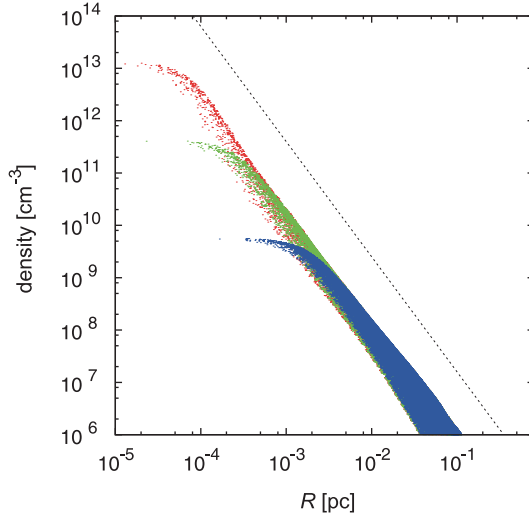


Fig. 4.4. Three snapshots at different times of radial distribution of the gas density in a minihalo. Cooled gas in a minihalo collapse in a runaway fashion to leave core-envelope structure with $\propto r^{-2.2}$ slope (dashed line denotes the slope for guiding the eye). The data were taken from the minihalo in the cosmological simulation of Ref. 31.

In fact, the collapse of cold gas in the minihalo found in the cosmological simulation proceeds in this way, as seen in Fig. 4.4, where the gas densities of SPH particles are plotted as a function of the distance from the density peak at three phases. A core and an envelope of $\propto r^{-2.2}$ form, which are consistent with the similarity solution [54]. Now, we go back to Fig. 4.3 to see the thermal processes along the evolutionary locus.

(A) Before this point, the cloud collapses adiabatically, and the temperature increases. After the temperature reaches ~ 1000 K, H_2 fraction becomes larger than $\sim 10^{-4}$, which is enough to cool the gas. This is the process essentially described in the previous section.

(B) Then the cloud cools rapidly via H_2 radiative cooling. The radiative cooling rate by H_2 is the line emission rate:

$$n_{\text{H}}n_{\text{H}_2}\Lambda_{\text{H}_2} \equiv \sum_{i < j} h\nu_{ji}A_{ji}n_{\text{H}_2,j}, \quad (4.17)$$

where $h\nu_{ji}$ is the energy gap between the i th and the j th levels, while A_{ji} denotes the spontaneous decay rate from the j th to the i th level. n_{H} and n_{H_2} denote the number density of the nuclei ($\simeq$ hydrogen atoms) and H_2 molecules. $n_{\text{H}_2,j}$ is the number density of H_2 at the j th level. The summation is taken for all possible pairs of transitions.

The number density of the H_2 at an excited level j is given by the equation of detailed balance,

$$\sum_i (A_{ji} + n_{\text{H}}C_{ji})n_{\text{H}_2,j} = \sum_i n_{\text{H}}n_{\text{H}_2,i}C_{ij}. \quad (4.18)$$

Here, C_{ij} and C_{ji} are the collisional excitation/de-excitation rate coefficients. In the low density limit, $A_{ji} \gg n_{\text{H}}C_{ji}$, H_2 number density in the excited state is given as $n_{\text{H}_2,j} = \sum_i n_{\text{H}}n_{\text{H}_2,i}C_{ij} / \sum_i A_{ji}$. Since the number density in the ground state ($i = 1$) is much larger than other levels, we only consider the ground state as the i th level for simplicity. Consequently, we obtain the cooling rate for low density limit as

$$n_{\text{H}}n_{\text{H}_2}\Lambda_{\text{H}_2}(n_{\text{H}} \rightarrow 0) \simeq n_{\text{H}}n_{\text{H}_2} \sum_j h\nu_{j1}C_{1j}. \quad (4.19)$$

Hence, the cooling rate per unit volume is proportional to the square of density, while Λ_{H_2} depends solely on the temperature that we have already seen as in Eq. (4.8).

On the other hand, for high density limit $A_{ji} \ll n_{\text{H}}C_{ji}$, the number density of H_2 in the excited state is obtained by the relation $\sum_i C_{ji}n_{\text{H}_2,j} = \sum_i C_{ij}n_{\text{H}_2,i}$. Thus, the ratios among the molecules at various energy levels are decided by local thermodynamic equilibrium (LTE), which depends only on the temperature. In this case, the cooling function is

$$n_{\text{H}}n_{\text{H}_2}\Lambda_{\text{H}_2} \simeq \sum_{j>i} \sum_i n_{\text{H}_2,i}h\nu_{ji}A_{ji}C_{ji} / \sum_i C_{ij}. \quad (4.20)$$

Consequently, the cooling rate per unit volume is proportional to the density. The LTE expression $\Lambda_{\text{H}_2}(\text{LTE})$ is complicated, but the readers can find it in Ref. 55.

Thus, the dependence of the cooling rate on the density changes at the critical density is defined as

$$n_{\text{cr}}C_{ji} \simeq A_{ji}. \quad (4.21)$$

The change of the total cooling rate occurs around 10^4 cm^{-3} by summing up the contribution from all transitions. In the low density limit, the cooling rate is proportional to n_{H}^2 and it is proportional to n_{H} in the high density limit.

In practice, we can use the cooling function defined as

$$\Lambda_{\text{H}_2} = \frac{\Lambda_{\text{H}_2}(\text{LTE})}{1 + \Lambda_{\text{H}_2}(\text{LTE})/\Lambda_{\text{H}_2}(n_{\text{H}} \rightarrow 0)}, \quad (4.22)$$

which covers the range involving the critical density.

(C) The gradient of the curve on $n_{\text{H}}-T$ plane (Fig. 4.3) changes its sign at the position marked as (C). The reason is as follows: the adiabatic heating time scale is proportional to the free-fall time, $(G\rho)^{-1/2}$, while the cooling time scale is

$$t_{\text{cool}} \propto \begin{cases} \rho^{-1} & \text{for } n_{\text{H}} \lesssim 10^4 \text{ cm}^{-3}, \\ \rho^0 & \text{for } n_{\text{H}} \gtrsim 10^4 \text{ cm}^{-3}, \end{cases} \quad (4.23)$$

because of the dependence of cooling rate on the density as described above. Thus, for $n_{\text{H}} \lesssim 10^4 \text{ cm}^{-3}$, the radiative cooling becomes more efficient than the compressional heating as the collapse proceeds, which makes the temperature decrease. In contrast, for $n_{\text{H}} > 10^4 \text{ cm}^{-3}$, the adiabatic heating rate increases faster than the cooling rate as the density increases. As a result, the temperature increases to make the cooling more effective and fill the gap of heating and cooling. Hence, we observe a dimple around 10^4 cm^{-3} . According to numerical simulations, the gas clouds are known to hesitate to collapse around 10^4 cm^{-3} because the equation of state of the gas becomes “stiff” beyond 10^4 cm^{-3} . Hence, the collapsing gas “loiter” around there, but it keeps cooling to proceed to further collapse.

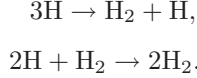
(I) The dashed curve represents the collapsing primordial gas with ionization by cosmic ray/radioactive elements of 0.01 times interstellar level. The ionization by cosmic ray/radioactive elements could play important roles in case we consider the environment of first galaxies [51, 56, 57]. Additional ionization leads to slightly abundant H_2 , which is the source of HD molecule formation via the following reaction:



As a result, abundance of HD increases. HD molecules are much more efficient coolants than H_2 , since they are antisymmetric molecules that allow dipole emission. Therefore the A-coefficient of rotational level transition is much larger than that of H_2 , which makes the radiative cooling as the HD rotational level transition becomes the dominant cooling process around the marked density range, although the amount of deuterium is much lesser than hydrogen. The rotational level transition from $j = 1$ to $j = 0$ is possible for HD, while $j = 2$ to $j = 0$ is the lowest transition level for H_2 . Moreover, the moment of inertia of HD is larger than H_2 because of the added neutron. Combining these facts, the lowest energy transition for HD is

128 K, which is four times lower than that of H_2 . This leads to the temperature of the collapsing gas less than 100 K in this case. It is worthwhile to note that another HD dominant cooling branch is found in the minihalos with relatively higher spin even without the additional ionization by cosmic rays/radioactive elements [32].

(D) After the cloud reaches $\sim 10^8 \text{ cm}^{-3}$, the following three-body reactions come into play:



Consequently, H_2 fraction increases rapidly above $\sim 10^8 \text{ cm}^{-3}$, thereafter most of the hydrogen atoms are converted into H_2 by the moment when the density goes beyond $\sim 10^{12} \text{ cm}^{-3}$. The abundant H_2 causes more efficient cooling of the gas, while at the same time, **(E)** the latent heat associated with the formation of H_2 is released. The energy is converted into the thermal energy of molecules, since the three-body reactions are not radiative processes. Thus, the H_2 formation process is an important heating process. Each reaction to form H_2 releases 4.48 eV, which is much larger than the thermal energy per molecules around this temperature, $\sim 1000 \text{ K}$. In fact, after the enhanced H_2 cooling becomes prominent, the gas temperature quickly recovers by the H_2 formation heating. As a result, the dip associated to the rapid increase of coolant, H_2 , is very shallow.

(F) Since the density and H_2 fraction increase rapidly, the H_2 rotational–vibrational line transitions become optically thick. In order to take into account the opacity of H_2 lines, we have to assess the optical depth of the lines. In one-dimensional radiation hydrodynamical calculations, the line transfer is solved directly [15], but not possible for multi-dimensional calculations. In three-dimensional calculations, Sobolev approximations are often used for three directions of the Cartesian coordinate. In these simulations, the optical depths along the three Cartesian axes are used to calculate the escape probabilities to the three directions. The three probabilities are averaged to give the emission rate from a certain fluid element [14, 58]. Another way to assess this effect is to use a fitting function, which simply depends on density [59, 60], although this simplification might cause errors in anisotropic structures.

(G) For yet higher densities of $> 10^{14} \text{ cm}^{-3}$, collision-induced emission (CIE) comes into play. Since the collision among H_2 molecules is so often at such high densities, H_2 collision pair stays in a transient state “supramolecule” for a while, where the electric dipole exists. The presence of the dipole moment allows either of the molecules to emit/absorb radiation more efficiently. H_2 starts to be disintegrated at $n_{\text{H}} \gtrsim 10^{16} \text{ cm}^{-3}$ subsequently. H_2 dissociation removes 4.48 eV per one molecule, which is the final process of primordial gas cooling. **(H)** Finally, for $n_{\text{H}} > 10^{20} \text{ cm}^{-3}$, collapse becomes almost adiabatic, followed by the formation of a protostar.

4.3.1. *Difference from the present-day star formation*

It is worthwhile to mention the difference between the thermal evolution of the collapsing primordial gas and the present-day counterpart. In Fig. 4.3, the dotted curve denotes the present-day case. It is obvious that the gas is much cooler than the primordial case, which is due to the presence of “metals” and dusts in the interstellar gas. However, for $n_{\text{H}} > 10^{10} \text{ cm}^{-3}$, the cloud becomes opaque by the dust opacity, thereby the collapse slows down and becomes nearly adiabatic. This phase (**J**) was called as the “first core” which plays important roles for the amplification of the magnetic field, launching the outflow from the protostar and formation of wide binaries. For very dense regions of $n_{\text{H}} > 10^{15} \text{ cm}^{-3}$, both tracks converge, since the metal lines and dust emission are not dominant cooling processes in such high densities. CIE cooling, H_2 dissociation cooling and the tail of the $\text{Ly}\alpha$ cooling are the dominant processes common in the primordial case.

4.3.2. *Lyman–Werner background radiation*

The very first stars are not affected by the radiative/kinetic effects of other stars, but as the stars are born hither and thither, ultraviolet radiation in the energy range of 11.26–13.6 eV is piled up to build the background radiation [61]. The radiation in this range is known as Lyman–Werner radiation, which contributes to dissociate the H_2 molecules. The impact of this background radiation on the Pop III star formation is quite significant [13, 62–65]. It is a self-regulative mechanism to keep the star formation rate from an explosive growth. Cosmological simulations found that if the intensity of the Lyman–Werner background radiation reaches $J_{\text{LW}} \lesssim 10^{-21} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1}$, star formation process in minihalos is strongly disturbed [32, 65]. Consequently, it also increases the minimal mass of the minihalo to host the cold star forming gas by an order of magnitude [13, 63, 66].

4.3.3. *Numerical techniques in the runaway phase*

In order to trace the birth of the proto-first-star by a numerical simulation, we have to solve the dynamics of the gas/dark matter starting from a cosmological initial condition, i.e., the hydrodynamics equations and equations of motion of dark matter particles with self-gravity. These equations have been solved both by Lagrangian and Eulerian schemes. Lagrangian schemes are almost equivalent to the Smoothed Particle Hydrodynamics (SPH) for gas motion, whereas Eulerian grid codes are also used. The N -body simulations are used to solve the motion of the dark matter particles. The representative example of the former designed for cosmological simulations is the series of GADGET [67, 68], and the ENZO [69–71] is for the latter. The intermediate scheme have also been developed, represented by the code AREPO [72]. AREPO is an Eulerian code with unstructured grids, but the grids move according to the flow of mass elements, thereby it is regarded as the intermediate between the Lagrangian scheme and the Eulerian one. All of

these codes have the advantage to zoom up tiny portions of the simulated volume by Particle Splitting technique for SPH and Adaptive Mesh Refinement for ENZO, and split the moving Voronoi mesh in AREPO. This feature is quite essential for the study on the first stars, since it requires a huge dynamic range from 10^{-2} cm^{-3} to 10^{20} cm^{-3} .

We also note that various thermal processes including chemical reactions, cooling/heating of gas have to be taken into account in this particular problem. In fact, the listed codes implement these features.

The chemical reactions have to be solved dynamically coupled with equation of motion/energy equation, since some reaction time scales are comparable with or longer than free-fall time or cooling time. Chemical reaction equations are written as follows in general:

$$\frac{dy_i}{dt} = \sum_j k_j y_j + n_H \sum_{k,l} k_{kl} y_k y_l + n_H^2 \sum_{m,n,s} k_{mns} y_m y_n y_s, \quad (4.25)$$

where y_i is the fraction of i th species, $y_i \equiv n_i/n_H$, with n_H being the number density of hydrogen nuclei, and k 's are the coefficients of reaction rates. These reaction rates are summarized in Refs. 47, 73, with the discussion on the accuracy of these rates. The solver of the rate equations has to be an implicit one, since some reaction time scales are very short compared with the others. Implicit solver always requires the matrix inversion, for which direct methods are used because the size of the matrix is $\sim 10 \times 10$.

4.4. Mass accretion phase

The hydrostatic core, i.e., the proto-first-star in the minihalo is tiny at its birth ($\sim 10^{-3} M_\odot$). However, plenty of gas are infalling onto it, thereafter the proto-first-star grows very rapidly. The mass accretion rate is $\sim c_s^3/G$, where c_s denotes the sound speed. As shown in Fig. 4.3, the temperature is much higher than that of the present-day counterpart, so is the accretion rate. In fact, the typical mass accretion rate in the nearby molecular cloud is $\sim 10^{-6}\text{--}10^{-5} M_\odot \text{ yr}^{-1}$, whereas the accretion rate in the primordial environment is $\sim 10^{-3}\text{--}10^{-2} M_\odot \text{ yr}^{-1}$. This rapid accretion corresponds to the rate at which the star grows to $10^2\text{--}10^3 M_\odot$ within 10^5 yrs . Since the mass of the host dense gas clump in the minihalo is $\sim 10^2\text{--}10^3 M_\odot$, it is possible for the proto-first-stars to grow up to $10^2\text{--}10^3 M_\odot$. Hence, as a first approximation, the typical mass of the first stars is well above the mass of the present-day stars. However, above arguments are very simplified because it ignores the formation and fragmentation of the accretion disk, and the radiative feedback in accordance with the evolution of the protostar, all of which have to be addressed. In this section, these processes are described, and the initial mass function (IMF) of the first stars is discussed at the end.

4.4.1. Evolution of the protostars

Evolution of proto-first-stars is quite important, since they could have UV feedback effect on the accretion flow depending on the evolutionary phase. Here, we show the typical evolution of these stars following the arguments in Refs. 18, 74.

Evolution of the proto-first-star is characterized by the following two time scales:

$$t_{\text{acc}} \equiv \frac{M_*}{\dot{M}_*}, \quad (4.26)$$

$$t_{\text{KH}} \equiv \frac{GM_*^2}{R_* L_*}. \quad (4.27)$$

The former denotes the mass accretion time scale, while the latter is the Kelvin–Helmholtz contraction time. Here, M_* , R_* , $\dot{M}_*$ are the mass and the radius of the protostar, and the mass accretion rate onto it. L_* denotes the luminosity of the radiation from the interior of the protostar.

As described in Section 4.3, the protostar is born at the center of the gravitationally contracting gas cloud, when the central density exceeds $\sim 10^{20} \text{ cm}^{-3}$. Just after the birth, the surrounding gas accretes very rapidly to release its gravitational energy as thermal energy at the shock on the surface of the star. In this initial phase, $t_{\text{acc}} < t_{\text{KH}}$ is satisfied because of the large mass accretion rate. Thus, the total luminosity of the protostar is dominated by the radiation from the shocked gas at the stellar surface, not by L_* . This phase is known and described as an adiabatic accretion phase.

The mass of the protostar gets larger with time. The increase of gravitational energy leads to a higher temperature of the stellar interior. As the temperature increases, the opacity of the gas decreases, since it is well approximated by Kramer’s opacity, $\kappa \propto \rho T^{-3.5}$. As a result, photons trapped in the interior of the protostar diffuse out of the star. Hence, L_* increases and t_{KH} gets shorter. L_* is dependent on the radius of the star and it peaks at a certain radius to give a maximum of L_* as

$$L_{\text{max}} \simeq 0.2 L_{\odot} \left(\frac{M_*}{M_{\odot}} \right)^{11/2} \left(\frac{R_*}{R_{\odot}} \right)^{-1/2}. \quad (4.28)$$

This is a result from numerical computation with $\dot{M}_* = 10^{-3} M_{\odot} \text{ yr}^{-1}$ [18], and its dependence is consistent with the luminosity of the contracting core with Kramer’s opacity [75].

On the other hand, the stellar radius in the adiabatic accretion phase is approximated as [76]

$$R_* \simeq 26 R_{\odot} \left(\frac{M_*}{M_{\odot}} \right)^{0.27} \left(\frac{\dot{M}_*}{10^{-3} M_{\odot} \text{ yr}^{-1}} \right)^{0.41}. \quad (4.29)$$

Hence, the stellar radius increases with stellar mass. Remark that R_* is quite large because of the huge mass accretion rate.

As the mass accretion proceeds, the stellar luminosity L_* keeps increasing to achieve $t_{\text{acc}} = t_{\text{KH}}$ eventually. This equality is satisfied when the stellar mass becomes

$$M_{*,\text{teq}} \simeq 14.9 M_{\odot} \left(\frac{\dot{M}_*}{10^{-2} M_{\odot} \text{yr}^{-1}} \right)^{0.26}. \quad (4.30)$$

This critical mass is obtained by the simultaneous equations of $t_{\text{KH}} = t_{\text{acc}}$ and $L_* = L_{\text{max}}$.

After passing this moment, $t_{\text{acc}} > t_{\text{KH}}$ is satisfied, and the stellar luminosity L_* is larger than the luminosity from the accretion shock. As long as the mass accretion rate is low enough to satisfy $\dot{M}_* < 0.01 M_{\odot} \text{yr}^{-1}$, the stellar radius starts to shrink. The protostar keeps collapsing until the central temperature reaches 10^7 K, at which the hydrogen burning starts, i.e., it settles down to the zero age main sequence (ZAMS). Majority of the proto-first-star evolve along this path that we have described above.

Figure 4.5 shows the evolution of the stellar radii as functions of M_* with various mass accretion rates [74]. For instance, in the case of $\dot{M} = 10^{-3} M_{\odot} \text{yr}^{-1}$, in the upper panel, we find that the stellar radius increases initially (adiabatic accretion phase) and it decreases in the later phase (KH contraction). The solid dots denote the ZAMS.

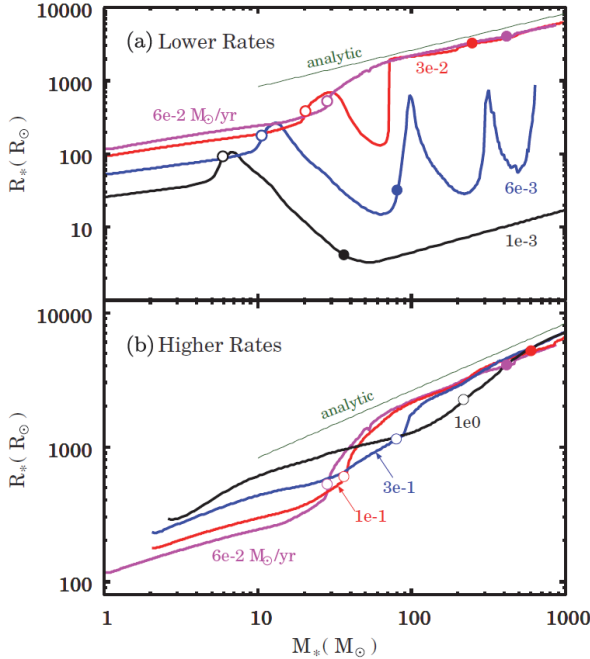


Fig. 4.5. Protostellar radii for various mass accretion rates as functions of the stellar mass [74].

On the other hand, in rare cases, very rapid mass accretion such that $\dot{M}_* > 0.01 M_\odot \text{yr}^{-1}$ is satisfied, the evolution of the stellar radius is very different. In Fig. 4.5, the cases of $\dot{M} = 3 \times 10^{-2} M_\odot \text{yr}^{-1}$ and higher mass accretion rates, the stellar radius do not turn to contraction even after $t_{\text{acc}} > t_{\text{KH}}$ is satisfied. In this phase, stellar interior contracts because t_{KH} is shorter than t_{acc} , but the accreted gas on the surface with the very large rate prevents the photons in stellar interior from escaping into the space. As a result, the outer part of the star is kept swelled up like red giants. Thus, the luminosity of the star increases as the mass accretion proceeds, but the radius is still very large. Consequently, the effective temperature of the protostar is low ($< 10^4 \text{K}$) which is not high enough to emit ultraviolet radiation. The absence of UV feedback results in no disturbance of mass accretion onto the protostar in these rare cases, which leads to the formation of very massive stars of $\gtrsim 10^3 M_\odot$.

4.4.2. Fragmentation of the accretion disk

The evolution of the protostar with a given spherical mass accretion rate was discussed in the previous section. However, in more realistic cases, the progenitor cloud has considerable angular momentum, thereby the mass accretion is not spherical, but form accretion disks. According to the cosmological simulation on the runaway phase of the first star formation, the specific angular momentum of the mass element at the final phase is ~ 0.5 times the Keplerian value [10, 14]. First, we try to assess the radius of the accretion disk.

Consider a mass element outside the runaway collapsing core. The distance from the center to the mass element is approximately given by the Jeans radius, r_J , calculated by the density/temperature of the gas element because the collapsing gas cloud converges to the Larson–Penston-type similarity solution. According to the numerical simulations and the similarity solution [77], the specific angular momentum of this element has ~ 0.5 times the Keplerian value. In the mass accretion phase, this element falls onto the disk at r_d to be rotationally supported. The conservation law of angular momentum reads

$$\sqrt{GM r_d} = 0.5 \sqrt{GM r_J}. \quad (4.31)$$

Thus, we have

$$r_d = 0.25 r_J. \quad (4.32)$$

Therefore, the mass element settles onto the rotationally supported disk when it falls only by a factor of four in radius.

The mass accretion rate is so high that the disk grows very rapidly. The stability of the disk can be understood by Toomre’s Q value, which is defined as

$$Q \equiv \frac{c_s \kappa}{\pi G \Sigma}, \quad (4.33)$$

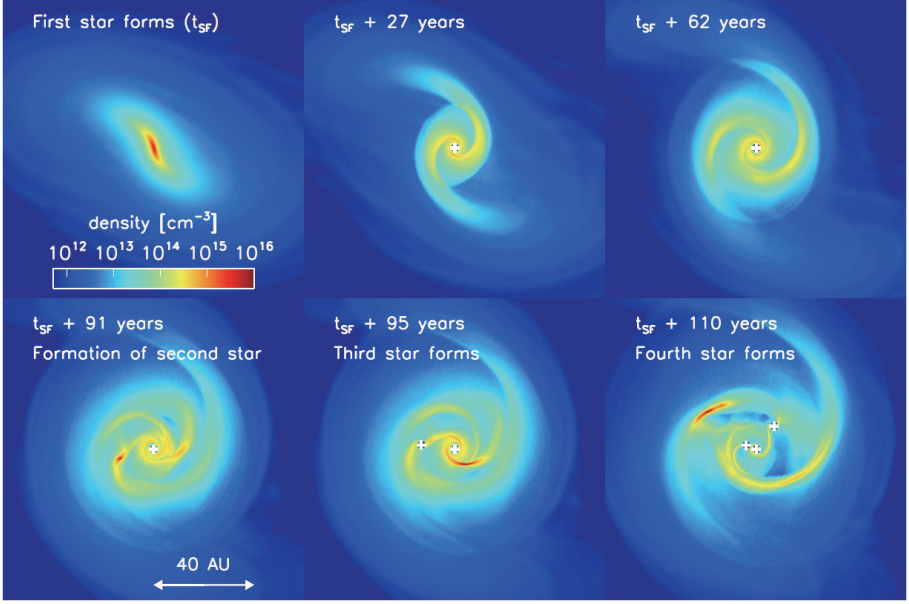


Fig. 4.6. The fragmentation of the accretion disk around a primary proto-first-star [78].

where κ denotes the epicyclic frequency (equal to the orbital angular velocity for Keplerian disk), c_s and Σ denote the sound velocity and the surface density of the disk, respectively. If Q is less than unity in a range of radius, the disk becomes gravitationally unstable. The accretion disks around first stars tend to be unstable because the large accretion rate onto the disk results in large Σ , thereby low Q . In nonlinear three-dimensional simulations, the regions where $Q < 1$ is satisfied emerge to develop spiral structures, thereafter the spiral arms fragment into clumps. Hence, the actual fragmentation process is highly nonlinear, which requires numerical simulations.

Two distinct types of simulations to investigate the nonlinear fragmentation process have been performed so far. The first group of works tries to achieve very high resolution in mass/length, utilizing zoom-in techniques [21, 24, 26]. They find that many fragmentations occur in the accreting disk. The fragments are self-gravitating and they collapse to the secondaries (Fig. 4.6). In these simulations, significant fraction of the fragments falls onto the primary and the rest of them survive during the simulated time, or get ejected from the high resolution simulated region. According to one of the highest resolution simulations [24], the survived fraction is $\sim 1/3$. However, the simulated time ($\lesssim 10\text{--}1000\text{yr}$, depending on the resolution) is much shorter than the entire evolutionary time of the protostar $\sim 10^5\text{yr}$. The fate of the “survived” secondaries are still uncertain.

Another group of simulations have less resolution than the former in order to trace much longer term. After longer time integration, disk radius becomes larger.

In addition, these simulations are required to implement the radiative feedback from the protostar, since the protostar becomes massive enough to emit UV photons after a few thousand years since the birth of the protostar. The effects of radiative feedback will be discussed in the next section. In these simulations, much larger disks are found, that also fragment into small pieces, but the fate of these clumps is not in agreement among the simulations so far [20, 27, 29, 31, 33, 34]. The simulations that utilize sink particle techniques predict a few — several stars form to survive [20, 27, 29, 31, 34], but grid code that simply assumes an adiabatic equation of state above a threshold density predicts that most of the fragments fall on to the primary [33]. This should be investigated in future researches.

4.4.3. Radiative feedback from the protostars

When the protostar grows above $\sim 15M_{\odot}$ and the mass accretion rate is lower than $\sim 10^{-2}M_{\odot}\text{yr}^{-1}$, the protostar shrinks via the Kelvin–Helmholtz contraction. Finally, the protostars settle down to the main-sequence phase to release a large amount of ultraviolet photons. The UV photons in the Lyman–Werner band (11.2–13.6 eV) take the lead in propagating into surrounding gas to dissociate H_2 molecules. H_2 dissociation diminishes the main coolant of the gas and also behaves as effective heating process coupled with the H_2 formation process [29]. After the sweep by LW radiation, ionizing radiation ($>13.6\text{ eV}$) follows to ionize the material especially in the polar direction because the gas density in the polar direction is $\sim 10^8\text{ cm}^{-3}$, which is much less dense than the gas at the inner edge of the disk. Thus, the emitted ionizing photons escape into the polar direction, gradually increasing the opening angle. Figure 4.7 shows the evolution of the temperature and density in a two-dimensional radiation hydrodynamic simulation that models the mass accretion phase of a first star formation [28]. The ionization fronts propagate into the polar directions initially. The Keplerian velocity at $\sim 100\text{ AU}$ is $\sim 10\text{ km s}^{-1}$, which is marginally not able to sustain the ionized gas of several $\times 10^4\text{ K}$. Hence, the ionized hot gas forms outflows into the poles, and the opening angle gradually increases since the ionizing radiation whittle away the gas by photoevaporation. As a result, the mass accretion rate rapidly decreases with time. In this particular case, the mass accretion totally stops when the mass of the star reaches $43M_{\odot}$. Other groups also perform radiation hydrodynamical simulation in 3D, they have also found that the final mass is less than $100M_{\odot}$ [20, 29].

Thus, the UV feedback is able to halt the mass accretion onto the first star, whose final mass is eventually determined. However, this final mass is obtained from one particular first star formation site, i.e., a minihalo. In order to obtain the typical mass/mass distribution of first stars, we have to perform this type of simulations from many initial conditions of minihalos. This will be discussed in the next section.

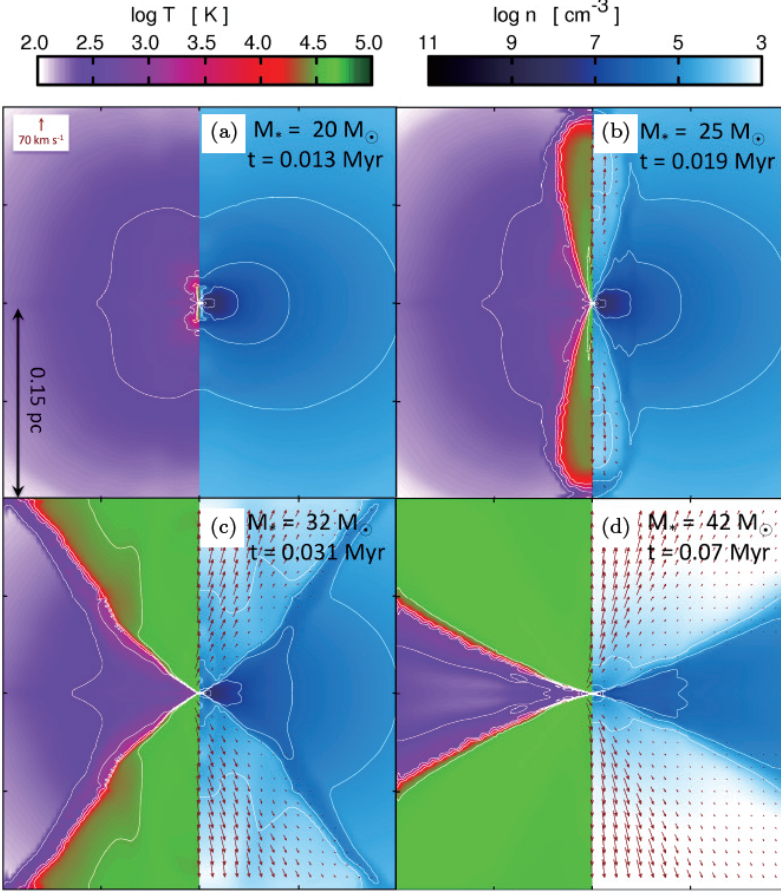


Fig. 4.7. Four snapshots of axisymmetric radiation hydrodynamical simulation of protostellar ultraviolet feedback [28]. The spatial distributions of gas temperature (left), number density (right), and velocity (right, arrows) are shown.

4.4.4. Final mass distribution of the first stars

As discussed in the previous section, UV feedback can halt the mass accretion onto the proto-first-stars. However, the host minihalos of those stars in cosmological context have some diversity. Hence, in order to obtain the distribution of the mass of the first stars, it is necessary to assess the final mass of the stars in various minihalos starting from cosmological initial conditions. In this section, we discuss the IMF of first stars based upon a theoretical consideration. Three groups have investigated this issue so far, although they have not converged yet.

In Ref. 30, cosmological simulations are performed in which ~ 110 cooling minihalos are found. They follow the runaway collapse phase of the cold gas in

these halos, thereafter they switch to the two-dimensional RHD grid code to trace the further evolution in the mass accretion phase by averaging along the azimuthal angle. As a result, they found that the mass in the final phase ($\sim 10^5$ yrs) at which the mass accretion almost halted spread from 10 to 1000 $M_\odot$. It is a very broad and top-heavy distribution. They also extended the work by performing large N -body simulation to pick up more than thousand minihalos [32]. They assume empirical relation between the final mass of the first stars and the mass accretion rate in the minihalos derived in the previous work. Consequently, even more top-heavy distribution than the previous calculation is obtained. On the other hand, these calculations are based on the two-dimensional simulations, which do not allow fragmentation of the accretion disk.

Ref. 27 has tackled this issue of fragmentation by simulating a few minihalos by three-dimensional calculation. They use SPH scheme coupled with radiative transfer of UV photons. Utilizing subgrid model to solve UV transfer in the very vicinity of the protostar, three-dimensional RHD simulations are achieved in which photoionization/photoheating are properly solved, although they could follow just 5000 yrs after the onset of the accretion phase. By extrapolating the results to $\sim 10^5$ yrs, they could obtain the final mass of the first star. In their simulations, the disk fragment into a few stars normally, and the mass is 10–40 solar masses. They also extended their work to higher resolution that resolves the inner 1AU region to find the fragmentation in the vicinity of the primary star. In fact, $\gtrsim 10$ fragments are found that might survive until the mass accretion ceases, but we have to keep in mind that the integrated time is 5000 yrs again. In Ref. 29, this issue is also studied using SPH scheme with radiative transfer (RSPH) [78]. They only could solve the transfer of LW photons because they do not take into account the subgrid model to trace the ionization front in the vicinity of the primary star. Picking up 59 minihalos from cosmological simulations, they perform three-dimensional RHD simulations to obtain the final mass distribution. Resultant mass distribution spread over from one to a few hundreds of solar masses again, although slightly less massive than the two-dimensional results [30, 32]. This difference could be originated from the fragmentation process, but still have possibilities that it stems from the difference of the numerical schemes. In fact, the accretion disk fragments commonly in Ref. 31, and two-third of the minihalos end up as multiple systems. However, Ref. 33 performs several RHD simulations in 3D grid code to find all of the fragments in the disk fall onto the primary star. The difference might have originated from the numerical scheme to handle the fragments, which should be addressed in the near future.

In this manner, the results of the theoretical studies on the Pop III IMF have not converged yet. Roughly speaking, all the calculations support a top-heavy IMF spread from ten to a few hundreds of solar masses, but there still remains large uncertainty on both the high and low-mass ends. In particular, the low-mass end could extend to much lower masses since higher resolution studies allow more low-mass fragments in the vicinity of the primary [34].

4.4.5. Numerical techniques in the mass accretion phase

In order to study the mass accretion phase, some new features have to be implemented to the code. First of all, the time step of the simulation becomes very short at the end of the mass accretion phase when the proto-first-star forms, since the size of the star is too small. The time step is so short that it is not possible to follow later evolution. Highest resolution simulation with no trick [24] can resolve 0.05 AU, which is much smaller than the protostellar radius, but it can trace only 10 yrs after the formation of the protostar. References 26, 79 use the barotropic equation of state instead, which is much less expensive than solving the energy equation. In addition, Ref. 26 uses the nested grids and Ref. 79 is a two-dimensional simulation, both also help to reduce the numerical costs dramatically.

Most of the researches with cosmological SPH simulation have employed the sink method, i.e., put sink particle that absorbs accreting mass, in which the internal structure is not solved [20, 21, 23, 25, 29]. Sink method usually assumes a threshold density and accretion radius. If the density of an SPH particle exceeds the threshold density, a sink particle is generated. The sink particle absorbs other SPH particles/sink particles if they are coming inside the accretion radius, and the additional conditions on energy [29] or angular momentum [20] are satisfied. These two parameters define the resolution of the simulation and the traceable span after the formation of the primary protostar.

On the other hand, in Ref. 33, radiative cooling is cut to avoid this sticking point when the simulation reaches the resolution limit. It also introduce a sink cell only for the primary protostar that allowed them to integrate up to $\sim 10^5$ yrs with radiative feedback.

4.5. Confrontation with Observations

Since the first stars form beyond $z \sim 10$, it is impossible to observe these stars directly even if they are very massive. However, we are able to obtain some constraints on the theory of the first star formation utilizing various remnants of those stars.

4.5.1. Abundance ratios in metal-poor systems

Metal-poor stars in Our Galactic halo could be born in the remnant of the “first supernova”, the supernova of an aged first star. The metallicity of these stars spread over a wide range, $-3 \lesssim [\text{Fe}/\text{H}] \lesssim -5$. In fact, the metallicity of the stars formed in the remnant of first stellar explosion is as low as $[\text{Fe}/\text{H}] = -3 \sim -4$ [80] and $[\text{Fe}/\text{H}] \sim -5$ for rare cases [81]. These are consistent with the observation of the metal-poor stars. Based upon the assumption that some fractions of the metal-poor stars are born in the remnant of first stars, the metal-poor stars should preserve the abundance ratio of the first stars. Therefore, we are able to approach the mass

of the first stars by observing the abundance ratio of these metal-poor stars. It is also possible to search the trace in the abundance of DLA systems since they are considered to be metal-deficient and forming galaxies.

According to the theoretical studies discussed in Section 4.4, a significant fraction of the first stars is very massive, exceeding $100M_{\odot}$. Thus, the evidence of such massive stars could be well expected. On the other hand, the stars within the mass range of $140M_{\odot}$ – $260M_{\odot}$ are expected to explode as pair instability supernovae (PISNe) [82]. Theoretically, these stars are known to have a strong “odd–even effect”, a remarkable deficiency of odd-charged nuclei compared to even-charged nuclei. Hence, it is little wonder that we find a trace of PISNe in the abundance pattern of metal-poor stars, but we have found no evidence of PISNe on the atmosphere of the stars with $[\text{Fe}/\text{H}] < -3$ so far. It is also worthwhile to note that the averaged abundance ratio of the metal-poor stars are consistent with the theoretical model of core-collapse supernovae [31] if we exclude the carbon enhanced metal-poor stars (CEMPs).¹ Considering the fact that more than 100 extremely metal-poor stars ($[\text{Fe}/\text{H}] < -3$) are already found in the Milky Way halo/dwarf galaxies, it is reasonable that the progenitors of these stars seem to be as massive as several tens of solar masses. Similar result is also obtained for DLA systems [31, 36, 37]. However, it is too hasty to conclude that no first stars formed in the mass range of $140M_{\odot}$ – $260M_{\odot}$. Since PISNe progenitors are so massive that they eject a large amount of heavy elements in a single explosion. Hence, the stars that form in the remnant of these stars could be pretty much enriched to the level of $[\text{Fe}/\text{H}] > -3$. In fact, Ref. 88 found a PISN candidate of $[\text{Fe}/\text{H}] = -2.5$. Search for the PISN abundance pattern among such “mildly” metal-deficient stars will provide more valuable information on the first star IMF.

4.5.2. *Hunting for the low-mass first stars*

In the previous section, we have discussed the observational constraint on the massive end of the Pop III IMF. On the other hand, we consider the constraint on the low-mass end in this section. As discussed in Section 4.4, the circumstellar disk form around the proto-first-stars, which is gravitationally very unstable. If a significant fraction of these fragments does not fall onto the central protostar to be excited to higher orbit of the stellar system or get ejected, they go through less dense regions of the accreting gas cloud. As a result, they are expected to remain less massive than the primary to evolve as low-mass stars. Hence, some fractions of the secondary first stars could be as massive as $\lesssim 1M_{\odot}$ in speculation. On the other hand, stars of $\lesssim 0.8M_{\odot}$ do survive until now, thus, we are able to find them as zero-metallicity stars (Pop III stars) if they exist. In turn, if we do not find any of them, the theoretical models, in which such low-mass first stars form, are excluded [89–91].

¹Several theoretical models for CEMPs are proposed [83–87].

Surveys of metal-poor stars have been scanned more than 10^5 stars in Our Galactic halo/dwarf galaxies. They found metal-deficient stars called as EMP stars (Extremely Metal Poor stars, $[\text{Fe}/\text{H}] < -3$), UMP stars (Ultra Metal Poor stars, $[\text{Fe}/\text{H}] < -4$) and HMP stars (Hyper Metal Poor stars, $[\text{Fe}/\text{H}] < -5$), but no Pop III star has been discovered so far. Only one HMP star with “normal” abundance ratio was found until mid of 2016 [92], although a CEMP star was found whose iron abundance is very low $[\text{Fe}/\text{H}] < -7$ [93]. These HMPs could be the surface-polluted Pop III stars [94]², but here, we employ a working hypothesis that such secondary metal accretion is not enough to soil the surface to the level of $[\text{Fe}/\text{H}] \simeq -5$ [93].

Theories can predict the expected number of Pop III stars that should be found in Our Galactic halo, based upon the Λ CDM cosmology. For instance, Ref. 91 predicted the number of survived Pop III stars utilizing a cosmological N -body simulation. They pick up minihalos that host the first stars and end up as parts of the Milky Way-sized halos. Assuming a simple model of low-mass star formation in minihalos, the position and luminosity of these stars that survive until present are traced by the N -body simulation plus a Pop III star formation/evolution model. Consequently, the distribution of survived Pop III stars in Our Galactic halo and thereby the probability to find them are obtained. Comparing the prediction with present observations, it is found that the model with one survivor per minihalo is marginally consistent with the present observations such as SEGUE, but 10 survivor model is very unlikely (but see Ref. 95). This means only a single low-mass star less than $0.8M_{\odot}$ is allowed to form from the gas cloud of $10^5M_{\odot}$ in the minihalo. In Ref. 90, this issue is also studied by the semianalytic scheme to conclude that the low-mass end of the Pop III IMF should be more massive than $0.68M_{\odot}$. In case we assume some HMP stars are polluted first stars, we only have two samples already found. Therefore, the observations still favor one survivor per minihalo model.

Hence, from the observations, the Pop III IMF seems to be very different from that in the present-day universe where most of the stars are born as subsolar stars as described by the Salpeter or Kroupa IMF. This fact strongly suggests that the star formation process in the primeval environment is very different from the present-day universe, supporting that the massive star formation is the dominant mode of the first star formation.

4.6. Issues to be addressed

4.6.1. Further numerical challenges

There have been two approaches to the first star formation simulations so far. First direction was to accomplish the very high resolution which enables to resolve even

²In Ref. 94, they discuss first stars that can be stained to the level of $[\text{Fe}/\text{H}] = -5$ in the minihalos. Therefore, “normal” HMP stars are potential candidates of survived first stars.

the protostellar radius. These simulations can trace the fragmentation of the accretion disk in the vicinity of the protostar, thereby it can trace the merging/ejection of these fragments, which would be crucial for the formation of low-mass stars. However, it can trace a very short duration $\lesssim 10^2\text{--}10^3$ yrs because of the very short time steps required for such high resolution simulations. Radiative feedback discussed in Section 4.4.3 come into play $\gtrsim 10^3$ yrs after the birth of the protostars, which is crucial for the determination of the final mass. Hence, we cannot obtain the final mass from such high resolution simulations at present.

On the other hand, using coarse resolution and relatively large accretion radius of the sink (~ 10 AU), we can proceed the calculation to much later physical time ($\sim 10^5$ yrs). It can implement the radiative feedback that limit the mass accretion and can obtain the final mass of the stars. However, in these simulations, we cannot trace the disk fragmentation within the accretion radius, which is probably important for the formation of low-mass stars.

It is difficult to improve this situation dramatically, but it is challenging to cover the above two phases by a single numerical simulation. Further numerical challenges are desired.

4.6.2. *Formation of the next generation stars*

Besides the formation of the very first stars, it is important to understand the formation mechanism of subsequent generation of stars, since they are considered to be the dominant population at the cosmic dawn. Various feedback mechanisms come into play, such as the radiative feedback from other stars, mechanical feedback of supernova explosions, and the chemical enrichment including the effects of dusts. All of these effects should be considered properly in order to understand the star formation rate/efficiency and the IMF of these stars. This topic is discussed in Chapters 2 and 5–7.

4.6.3. *Magnetic field*

Most unknown part of the present first star formation theory is the magnetic field. In the present-day star forming regions, the magnetic energy density is comparable to the kinetic/thermal/gravitational energies. On the other hand, B-field has been considered to be absent in the first star formation sites in the early universe, since the age of the universe is too short for the B-field to be amplified enough. However, it is proposed that turbulent motion in the minihalos can drive the small-scale dynamo action, which rapidly amplifies the B-field to be a dynamically significant level. Under the presence of such a tense magnetic field, it has an unyielding impact on the first star formation: the outflows are launched at the end of the runaway collapse phase [96], and the disk fragmentation would be suppressed in the accretion phase. In other words, we have to consider the presence/effects of magnetic field seriously if it exists.

Minihalos are found at the nodes of the cosmic web as seen in Fig. 4.2 along with the gas/dark matter flow injecting into the minihalos. The kinetic energy of this inflow activates the turbulent motion of gas. The kinetic motion arises at the Jeans scale ℓ_J ($\simeq$ the length scale of minihalos), and it is expected to cascade down to the tinier scales because of the large Reynolds number.

The smallest scale of the turbulence is the viscous scale at which $\ell_{\text{vis}} v_{\text{vis}} \simeq \nu$ is satisfied. Here, ν denotes the kinetic viscosity of gas. The typical turbulent flow velocity v at a scale ℓ is proportional to $v \propto \ell^\vartheta$, where ϑ is in the range of $1/3 - 1/2$, depending on the compressibility of the flow. Using the Reynolds number, Re , the ratio of the viscous scale to the Jeans scale is given as $\ell_{\text{vis}}/\ell_J \simeq Re^{-1/(\vartheta+1)}$. On the other hand, the Reynolds number of minihalos at $\sim 1 \text{ cm}^{-3}$ is $Re \simeq 10^6$. Consequently, we have $\ell_{\text{vis}}/\ell_J \simeq 10^{-4} - 10^{-5}$ at $\sim 1 \text{ cm}^{-3}$.

The eddy time scale of the turbulent motion at the viscous scale is much shorter than other time scales, e.g., the free-fall time, since this scale is much smaller than the Jeans scale. In fact, the ratio of the eddy time scale at the viscous scale to the time scale at Jeans scale is given as

$$\frac{\tau_{\text{vis}}}{\tau_J} = \left(\frac{\ell_{\text{vis}}}{\ell_J} \right)^{1-\vartheta} \ll 1. \quad (4.34)$$

Thus, the magnetic field grows much faster at the viscous scale than the Jeans scale, since the eddy time scale is almost equivalent to the growth time scale. The amplified magnetic energy at the small scales flow into larger scales via the mode coupling effects embedded in the induction equation. Finally, the magnetic energy is comparable to the equipartition level even at the Jeans scale.

The above theory of B-field amplification in the minihalos has been discussed by analytic/numerical methods. The analytic model is based upon the Kazantsev–Kraichnan equation, which describes the time evolution of the two-point correlation function of the B-field in the kinetic limit, where the magnetic energy is negligible compared with the turbulent energy [97–99]. In Ref. 99, the equation is solved as an eigenvalue problem to find that the B-field grows exponentially if the magnetic Reynolds number $Rm \equiv R_J c_s / \eta$ satisfies $Rm \gtrsim 100 - 2000$, depending on ϑ . Here, η denotes the resistivity of the gas. It is also pointed out that the minihalos satisfy the condition of the exponential growth.

However, this very rapid growth has not been proved by numerical experiments, since the Reynolds number of the system is too large to resolve the viscous scale in the collapse simulations of minihalos. In fact, it requires MHD simulations of $\sim 100000^3$ at $\sim 1 \text{ cm}^{-3}$, which is beyond the capability of state-of-art supercomputers.

Based upon the current status described above, numerical simulations have been discovered following facts, although they have much coarser resolution than ℓ_{vis} [100–103]. First of all, the growth of B-field by the turbulence does exist in the collapsing minihalos, but it requires at least 32 grids to resolve the Jeans length. It

is also worthwhile to note that the amplitude of the B-field does not converge, i.e., to the finer resolution, the larger the magnetic field strength we get. Secondly, if we decompose the B-field distribution into Fourier components, we see an evidence of inverse cascading of magnetic field energy from the smallest scale to larger scales. All of these results are consistent with the results from the analytic calculations.

Nevertheless, we have to keep in mind that no simulation has shown the growth of magnetic field to the level of equipartition via the turbulent dynamo in the minihalos, starting from the realistic, very weak seed field of $\lesssim 10^{-18}$ G. This is simply due to the lack of resolution in the current simulations.

We also have to keep in mind that the turbulence of the collapsing minihalos in cosmological simulations has not been quantified enough to discuss the small-scale dynamo. It could be turbulent, but how the kinetic energy is supplied from the inflow along the cosmic web is still unknown.

Thus, the small-scale dynamo in the minihalo seems to be present, but we still have a few steps to confirm its significance.

4.7. Summary

In this chapter, theoretical models of the first star formation as well as the observational evidence, although they are not sufficient so far, are described. Based upon the Λ CDM cosmology, the first stars are born in the minihalos whose masses are $\sim 10^6 M_\odot$ at $z \sim 20$ –30, and the majority of the stars fall in the range of 10 – $1000 M_\odot$. In addition, the fragmentation process of the circumstellar disk around the proto-first-star could lead to the formation of much less massive stars that might survive until the present, while the actual survival rate is still very uncertain due to the limited resolution of the numerical simulations.

Observations of the metal-poor systems prefer the mass range of $10 M_\odot \lesssim M \lesssim 100 M_\odot$, but little evidence is found for more massive ones which end up as PISN. No metal-free stars have been found so far, which could constrain the low-mass end of the mass distribution of first stars.

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Chapter 5

First Galaxies and Massive Black Hole Seeds*

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One of the exciting frontiers of modern cosmology is to understand the emergence of the first sources of light, galaxies and accreting supermassive black holes during the first billion years of cosmic history. To provide a heuristic map for the impressive array of upcoming next-generation observational facilities, among them the *James Webb Space Telescope (JWST)*, ever more realistic numerical simulations play a key role. In this chapter, we will discuss some of the basic principles that govern first galaxy formation and the challenges they present for the simulation field. Prime among them is the proper treatment of the feedback effects exerted by the first (Population III) stars, including radiative and supernova feedback. A closely related problem is the formation of the first massive seed black holes, whose X-ray feedback could significantly impact the assembly process of the first galaxies. In conclusion, we will briefly survey the prospects for empirically testing our emerging theoretical framework.

5.1. Introduction

When did galaxies and supermassive black holes (BHs) first appear on the cosmic scene? How did the first stars transform the early universe from the simple initial state of the cosmic dark ages into one of ever-increasing complexity? For comprehensive reviews of this fundamental transition, see Refs. [3–6]. This process began with the formation of the first stars, the so-called Population III (Pop III), at redshifts $z \sim 20\text{--}30$. These stars are predicted to form in dark matter (DM) minihalos, comprising total masses of $\sim 10^6 M_\odot$. Current models suggest that Pop III stars were typically massive, or even very massive, with $M_* \sim 10\text{--}100 M_\odot$; these models also predict that the first stars formed in small groups, including binaries or higher-order

*This is based on two previous publications of the author [1, 2].

multiples. First star formation has been reviewed in Refs. [7, 8], where key papers are surveyed up to 2005, and in Refs. [2, 9], where the subsequent developments are discussed. In addition, for the most recent simulation results, beginning to push into the late stages of protostellar accretion, where radiation hydrodynamics becomes important, see the specialized literature (e.g., [10, 11]).

Once the first stars had formed, feedback processes began to modify the surrounding intergalactic medium (IGM). It is useful to classify them into three categories (see Ref. [12]): radiative, mechanical, and chemical. Here, radiative feedback consists of the hydrogen-ionizing photons emitted by Pop III stars, as well as the less energetic, molecule-dissociating radiation in the Lyman–Werner (LW) bands. Once the first stars die, after their short life of a few million years, they will explode as a supernova (SN) or directly collapse into BHs. In the SN case, mechanical and chemical feedback come into play. The SN blastwave exerts a direct, possibly very disruptive, feedback on its host system, whereas the chemical feedback acts in a more indirect way, as follows: The first stars, forming out of metal-free, primordial gas, are predicted to be characterized by a top-heavy initial mass function (IMF). Once the gas has been enriched to a threshold level, termed “critical metallicity” (Z_{crit}), the mode of star formation reverts to a more normal IMF, which is dominated by lower mass stars (see Refs. [13–15]). Chemical feedback refers to this transition in star formation mode, implying that less massive stars have a less disruptive impact on their surroundings. The complex physics of pregalactic metal enrichment, and the nucleosynthesis in Pop III SNe, are comprehensively reviewed in Ref. [16].

The formation environment for the first, Pop III, stars is provided by minihalos with their shallow gravitational potential wells. As these stars were typically very massive, they would quickly exert a strong negative feedback on their host systems. Numerical simulations indicate that this feedback completely destroys the host in the sense of heating and evacuating all remaining gas. There would therefore be no opportunity for a second burst of star formation in a minihalo. Furthermore, since all (most?) Pop III stars are massive enough to quickly die, there would be no long-lived system of low-mass stars left behind. The Pop III forming minihalos, therefore, are *not* galaxies in the usual sense if a bonafide galaxy is meant to imply a long-lived stellar system, embedded in a DM halo. The question, *What is a galaxy, and, more specifically, what is a first galaxy?*, however, is a matter of ongoing debate (see Ref. [17]), and as we have seen, this question is intimately tied up with the feedback from the first stars, which in turn is governed by the Pop III IMF (top-heavy or normal).

Theorists have been exploring the hypothesis that “atomic cooling halos” are viable hosts for the true first galaxies [18]. These halos have deeper potential wells, compared to the minihalos mentioned above; indeed, they have “virial temperatures” of $T_{\text{vir}} \simeq 10^4$ K, enabling the primordial gas to cool via efficient line emission from atomic hydrogen. We will further clarify these concepts below. It is useful to keep in mind that observers and theorists often employ different definitions.

As a theorist, you wish to identify the first, i.e., lowest-mass, DM halos that satisfy the conditions for a galaxy. Observers, on the other hand, usually aim at detecting truly metal-free, primordial systems. Recent simulation results, however, suggest that such metal-free galaxies may not exist. The reason being that rapid SN enrichment from Pop III stars, formed in the galaxy’s minihalo progenitors, provided a bedrock of heavy elements. Any second generation stars would then already belong to Population II (Pop II). These questions, and the problem of first galaxy formation in general, have been reviewed in Refs. [4, 5], where the reader can again find pointers to the detailed literature. For a comprehensive overview of galaxy formation and evolution in general, including the situation at lower redshifts, $0 < z < 5$, see Ref. [19], which is particularly good in discussing the large-scale aspects of galaxy formation.

The first star and galaxy field is just entering a dynamic phase of rapid discovery. This development is primarily driven by new technology, on the theory side by ever more powerful supercomputers, reaching peta-scale machines, and on the observational side by next-generation telescopes and facilities. Among them are the *James Webb Space Telescope (JWST)*, to be launched in ~ 2018 , and the suite of extremely large, ground-based telescopes, such as the Giant Magellan Telescope (GMT), the Thirty Meter Telescope (TMT), and the European Extremely Large Telescope (E-ELT). The capabilities of the *JWST* are summarized in Refs. [20, 21]. Complementary to these optical and near-infrared telescopes are recently commissioned and future meter-wavelength radio arrays, designed to detect the redshifted 21 cm radiation from the neutral hydrogen in the early universe (see Ref. [22]). Another intriguing window into the epoch of the first stars is provided by high-redshift gamma-ray bursts (GRBs). These are extremely bright, relativistic explosions, triggered when a rapidly rotating massive star is collapsing into a BH (see Ref. [23] for a broad introduction). The first stars are promising GRB progenitors, thus possibly enabling what has been termed “GRB cosmology” (for details, see Refs. [24, 25]).

There is a second approach to study the ancient past, nicely complementary to the *in situ* observation of high-redshift sources. This alternative channel, often termed “Near-Field Cosmology” [26], is provided by local fossils that have survived since early cosmic times. Among them are extremely metal-poor stars found in the halo of the Milky Way. The idea here is to scrutinize their chemical abundance patterns and derive constraints on the properties of the first SNe, and, indirectly, of the Pop III progenitor stars, such as their mass and rate of rotation (for reviews, see Refs. [27, 28]). Another class of relic objects is made up of the newly discovered extremely faint dwarf galaxies in the Local Group. These ultra-faint dwarf (UFD) galaxies consist of only a few hundred stars and reside in very low-mass DM halos. Their chemical and structural history is therefore much simpler than what is encountered in massive, mature galaxies, and it should be much more straightforward to make the connection with the primordial building blocks (e.g., Ref. [29]).

The plan for this chapter is to provide a broad-brush overview, focusing on the basic physical principles that constitute the foundation to understand the end of the cosmic dark ages. We will consider the overall cosmological context, the fundamentals of star formation as applicable to the primordial universe, the physical principles underlying the assembly of the first galaxies, and the emergence of the first BHs. We conclude with some useful tools of observational cosmology, allowing us to connect theory with empirical probes.

5.2. The cosmological context

5.2.1. Cold dark matter structure formation

We now have a very successful model that describes the expansion history of the universe and the early growth of density fluctuations (e.g., [31, 32]). This is the Λ cold dark matter (Λ CDM) model, as calibrated with high precision by the *Wilkinson Microwave Anisotropy Probe* (*WMAP*) and the *Planck* mission. Recently, a number of alternative models for structure formation have received renewed attention. All of them tend to address various problems of Λ CDM on small scales by postulating properties of the unknown DM particle that would act to suppress small-scale structures. Among them are traditional warm dark matter (WDM) models, light axion-based, or wavelike DM scenarios, such as fuzzy dark matter (FDM), and self-interacting DM models. It is currently not clear whether there is really a need for such a nonstandard approach, given that baryonic feedback processes might be able to account for the small-scale suppression. Improved simulations of galaxy formation, astronomical observations, and particle physics experiments might soon guide us to a deeper understanding of the true nature of DM and thus towards the correct model of cosmological structure formation.

Within Λ CDM, structure formation proceeds hierarchically, in a bottom-up fashion, such that small objects emerge first and subsequently grow through mergers with neighboring objects and the smooth accretion of matter. To characterize the resulting distribution of density fluctuations, we measure the “overdensity” in a spherical window of radius R and total (gas + dark matter) mass M , where $M = 4\pi/3\bar{\rho}R^3$:

$$\delta_M \equiv \frac{\rho - \bar{\rho}}{\bar{\rho}}. \quad (5.1)$$

Here, ρ is the mass density within a given window, and $\bar{\rho}$ that of the background universe at the time the overdensity is measured. Next, the idea is to place the window at random everywhere in the universe and to calculate the (mean-square) average: $\sigma^2(M) = \langle \delta_M^2 \rangle$, where the brackets indicate a spatial average. The latter is closely related to the ensemble average, where one considers many realizations of the underlying random process that generated the density fluctuations in the very early universe (ergodic theorem). Here and in the following, all spatial scales are physical, as opposed to comoving, unless noted otherwise.

Due to gravity, the density perturbations grow in time. This growth is described with a “growth factor,” $D(z)$, such that

$$\sigma \propto D(z) \propto a = \frac{1}{1+z}. \quad (5.2)$$

The second proportionality is only approximate and would be strictly valid in a simple Einstein–de Sitter background model. The expression for the growth factor is more complicated in a Λ -dominated universe (see Refs. [5, 19]), but the Einstein–de Sitter scaling still gives a rough idea for what is going on at $z \gg 1$. Indeed, it is quite useful for quick back-of-the-envelope estimates. Early on, all fluctuations are very small, with $\delta_M \ll 1$; but at some point in time, a given overdensity will grow to order unity. One says that a fluctuation is in its linear stage, as long as $\delta_M < 1$, and becomes “nonlinear” when $\delta_M > 1$. Formally, a critical overdensity of $\delta_c = 1.69$ is often used to characterize the transition. The behavior and evolution of the perturbations in their linear stage can be treated analytically, e.g., by decomposing a density field into Fourier modes. Once the fluctuation turns nonlinear, one needs to resort to numerical simulations to further follow them to increasingly high densities.

A basic tenet of modern cosmology is that the quantum-mechanical processes that imprinted the density fluctuations in the very early universe left behind a (near-) Gaussian random field. The probability that an overdensity has a given value, around a narrow range $d\delta_M$, is then

$$P(\delta_M)d\delta_M = \frac{1}{\sqrt{2\pi\sigma_M^2}} \exp\left[-\frac{\delta_M^2}{2\sigma_M^2}\right] d\delta_M. \quad (5.3)$$

One speaks of a “ ν -sigma peak,” when $\delta_M = \nu\sigma_M$. Note that high-sigma peaks are increasingly unlikely and therefore rare. One also says that such peaks are highly biased, and one can show that such peaks are strongly clustered (see, e.g., Ref. [19]). The sites for the formation of the first stars and galaxies are predicted to correspond to such high-sigma peaks. To predict the redshift of collapse, or “virialization” redshift (see below), we demand $\delta_M(z) = D(z)\delta_M(z=0) \simeq \delta_c$, or, using Eq. (5.2),

$$\frac{\nu\sigma_M(z=0)}{1+z_{\text{vir}}} \simeq 1.69,$$

such that $1+z_{\text{vir}} \simeq \nu\sigma_M(z=0)/1.69$, where $\sigma_M(z=0)$ is the rms density fluctuation, extrapolated to the present. On the scale of a minihalo ($M \sim 10^6 M_\odot$), one has $\sigma_M(z=0) \sim 10$. For collapse (virialization) to occur at, say, $z_{\text{vir}} \simeq 20$, we would then need $\nu \simeq 3.5$. Thus, the first star forming sites are rare, but not yet so unlikely to render them completely irrelevant for cosmic history.

5.2.2. *Virialization of DM halos*

Once a given perturbation becomes nonlinear ($\delta_M \sim 1$), the corresponding DM collapses in on itself through a process of violent dynamical relaxation. The rapidly changing gravitational potential, $\partial\varphi/\partial t$, acts to scatter the DM particles, and their

ordered motion is converted into random motion. The result of this “virialization” is a roughly spherical halo, where the kinetic and gravitational potential energies approach virial equilibrium: $2E_{\text{kin}} \simeq -E_{\text{pot}}$. Note that the total energy, $E_{\text{tot}} = E_{\text{kin}} + E_{\text{pot}} = -E_{\text{kin}}$, is negative, which implies that the halo is bound.

It is now convenient to define the gravitational potential (potential energy per unit mass) as follows:

$$\varphi = \frac{E_{\text{pot}}}{M_{\text{h}}} \simeq -\frac{GM_{\text{h}}}{R_{\text{vir}}}. \quad (5.4)$$

Here, M_{h} is the halo mass (gas + DM), which is connected to the halo density and radius, often called “virial” density and radius, via

$$M_{\text{h}} \simeq \frac{4\pi}{3} \rho_{\text{vir}} R_{\text{vir}}^3. \quad (5.5)$$

The virial density, established after the virialization process is complete, is related to the background density of the universe at the time of collapse, at z_{vir} : $\rho_{\text{vir}} \simeq 200\bar{\rho}(z_{\text{vir}})$. In terms of the present-day background density, one has

$$\bar{\rho}(z) = (1+z)^3 \bar{\rho}(z=0) = 2.5 \times 10^{-30} \text{ g cm}^{-3} (1+z)^3. \quad (5.6)$$

A very useful concept to gauge how the baryonic (gaseous) component will behave when falling into the DM halos mentioned above is the “virial temperature”. The idea is to ask what would happen to a proton, of mass $m_{\text{H}} = 1.67 \times 10^{-24} \text{ g}$, when it is thrown into such a DM potential well. Through compressional heating, either adiabatically or involving shocks, the particle would acquire a random kinetic energy of

$$k_{\text{B}} T_{\text{vir}} \simeq \epsilon_{\text{kin}} \simeq -\epsilon_{\text{pot}} \simeq \frac{GM_{\text{h}} m_{\text{H}}}{R_{\text{vir}}}, \quad (5.7)$$

where k_{B} is Boltzmann’s constant. Combining the equations above yields

$$T_{\text{vir}} \simeq 10^4 \text{ K} \left(\frac{M_{\text{h}}}{10^8 M_{\odot}} \right)^{2/3} \left(\frac{1+z_{\text{vir}}}{10} \right), \quad (5.8)$$

where the normalizations are appropriate for a first-galaxy system, or, technically, an atomic cooling halo. For a minihalo, where $M_{\text{h}} \sim 10^6 M_{\odot}$ and $z_{\text{vir}} \sim 20$, one has $T_{\text{vir}} \sim 1,000 \text{ K}$. A related quantity is the halo binding energy

$$E_{\text{b}} \simeq |E_{\text{tot}}| \simeq \frac{1}{2} \frac{GM_{\text{h}}^2}{R_{\text{vir}}} \simeq 10^{53} \text{ erg} \left(\frac{M_{\text{h}}}{10^8 M_{\odot}} \right)^{5/3} \left(\frac{1+z_{\text{vir}}}{10} \right), \quad (5.9)$$

where the normalizations are again appropriate for an atomic cooling halo. For a minihalo, the corresponding number is $E_{\text{b}} \sim 10^{50} \text{ erg}$. Comparing these values with the explosion energy of Pop III SNe, where $E_{\text{SN}} \simeq 10^{51} - 10^{52} \text{ erg}$, one gets

the zeroth-order prediction that minihalos may already be severely affected by SN feedback, evacuating most of the gas from the DM halo (see Ref. [12]). The more massive atomic cooling halos, on the other hand, are expected to survive such negative SN feedback. This expectation is roughly born out by numerical simulations (see Ref. [4]).

5.2.3. Gas dissipation

To form something interesting, such as stars, BHs, or galaxies, gas needs to be able to collapse to high densities. Initially, such collapse is triggered by the DM potential well in halos, as the DM is dynamically dominant, and the gas (the baryons) just follows along. However, different from DM, the gas is collisional and therefore subject to compressional heating. If this heat could not be radiated away, or dissipated, there would eventually be sufficient pressure support to stop the collapse. The key question then is: *Can the gas sufficiently cool?* A simple, but intuitively appealing and useful, answer is provided by the classical Rees–Ostriker–Silk criterion that the cooling time has to be shorter than the free-fall time: $t_{\text{cool}} < t_{\text{ff}}$. If this criterion is fulfilled, a gas cloud will be able to condense to high densities and possibly undergo gravitational runaway collapse. These important time scales are defined as follows: $t_{\text{ff}} \simeq 1/\sqrt{G\rho}$ and $t_{\text{cool}} \simeq nk_{\text{B}}T/\Lambda$, where Λ is the cooling function (in units of $\text{erg cm}^{-3} \text{s}^{-1}$).

In Fig. 5.1, the cooling function for primordial, pure H/He, gas is shown (see also Chapters 3 and 6). One can clearly distinguish two distinct cooling channels, one at $T > 10^4 \text{ K}$, where cooling relies on atomic hydrogen lines, and one at lower temperatures, where the much less efficient H_2 molecule is the only available coolant. In the present-day interstellar medium (ISM), metal species would dominate cooling in this low-temperature regime, but, by definition, they are absent in the primordial universe. The first cooling channel governs the formation of the first galaxies (atomic cooling halos), since $T_{\text{vir}} \sim 10^4 \text{ K}$ for $M_{\text{h}} \sim 10^8 M_{\odot}$ and $z_{\text{vir}} \sim 10$. First star formation in minihalos, on the other hand, is governed by the low temperature, H_2 , cooling channel. The reason is again that minihalos typically have $T_{\text{vir}} \sim 1000 \text{ K}$.

5.2.4. Halo angular momentum

Another important ingredient for early star and galaxy formation is angular momentum. Current cosmological models posit that the post-recombination universe, at $z < 1000$, was free of any circulation ($\nabla \times \vec{v} = 0$). Angular momentum is thought to have been created through tidal torques during the collapse of slightly asymmetric overdensities. The idea is that neighboring perturbations exert a net torque on a given halo, thus spinning it up. It is convenient to parameterize the resulting total angular momentum, J , of a virialized halo by a “spin parameter”:

$$\lambda \equiv \frac{J|E_{\text{tot}}|^{1/2}}{GM_{\text{h}}^{5/2}} \simeq \left(\frac{E_{\text{rot}}}{|E_{\text{tot}}|} \right)^{1/2}, \quad (5.10)$$

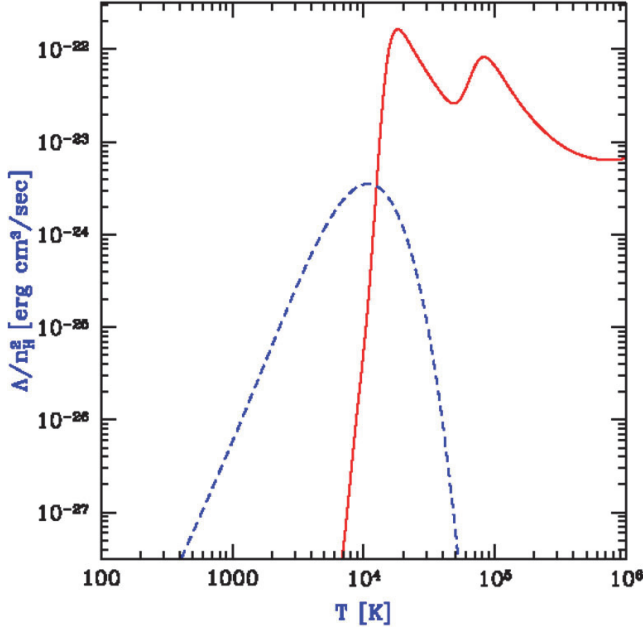


Fig. 5.1. Cooling rate of primordial gas as a function of temperature. Shown is the contribution from atomic hydrogen and helium (*solid line*), as well as that from molecular hydrogen (*dashed line*). Atomic hydrogen line cooling is very efficient at temperatures of $T > 10^4$ K, whereas at lower temperatures, cooling has to rely on H_2 , which is a poor coolant. This is the regime of the minihalos, hosting the formation of the first stars. Adapted from Ref. [30].

where $|E_{\text{tot}}|$ is again the total halo (binding) energy, and $E_{\text{rot}} \simeq J^2/(M_h R_{\text{vir}}^2)$ the total rotation energy. Numerical simulations, studying the large-scale evolution of the DM component, have shown that the spin parameter is distributed in a log-normal fashion with a mean of $\bar{\lambda} \simeq 0.04$ (see Ref. [19]).

For the DM component, the spin parameter is conserved during collisionless evolution. During the dissipational collapse of the gas, however, the spin parameter can change. In particular, the system can be driven towards centrifugal support, where $E_{\text{rot}} \simeq |E_{\text{tot}}|$. *What is the radius of centrifugal support?* Assume that the baryons collapse further in a fixed DM halo potential. It is then straightforward to show that the baryons have to collapse by a factor of $\sim \lambda^{-1}$ to reach centrifugal support: $R_{\text{cent}} \simeq \lambda R_{\text{vir}}$. This then is the typical dimension of any large-scale disk that forms inside a DM halo.

5.3. Primordial star formation

Primordial star formation shares many similarities with the present-day case in terms of basic principles. It is therefore always a good idea to seek guidance from the rich phenomenology and understanding reached in classical star formation theory

(see Refs. [33–35] for reviews). In the following, in the spirit of our basic toolkit approach, we will address gravitational (Jeans) instability, the physics of protostellar accretion, and the general properties of the stellar IMF.

5.3.1. Gravitational instability

Consider a gaseous cloud of linear size L with a given mass density ρ and temperature T . Such a cloud will be unstable to gravitational runaway collapse if $t_{\text{sound}} > t_{\text{ff}}$, with $t_{\text{sound}} \simeq L/c_s$ being the sound-crossing time. The sound speed is $c_s \simeq \sqrt{k_B T/m_H} \propto T^{1/2}$. The intuition here is that the free-fall time measures the strength of gravity in the sense that a smaller t_{ff} corresponds to a stronger force of gravity. Similarly, the sound-crossing time scale provides a measure for the strength of the opposing thermal pressure, where again a smaller t_{sound} indicates stronger pressure forces. The above time-scale criterion for gravitational instability can be written as

$$\frac{L}{c_s} > \frac{1}{\sqrt{G\rho}}. \quad (5.11)$$

This inequality defines the Jeans length

$$L > L_J \simeq \frac{c_s}{\sqrt{G\rho}}, \quad (5.12)$$

with the interpretation that a density perturbation has to exceed a certain critical size, such that gravitational forces take over, and cannot be balanced by thermal pressure any longer. One then defines the *Jeans mass* as follows:

$$M_J \sim \rho L_J^3 \simeq 500 M_\odot \left(\frac{T}{200 \text{ K}} \right)^{3/2} \left(\frac{n}{10^4 \text{ cm}^{-3}} \right)^{-1/2}, \quad (5.13)$$

where $n \simeq \rho/m_H$ is the hydrogen number density, and the normalizations reflect typical values in Pop III star forming regions. A closely related concept is the *Bonnor–Ebert mass*, where $M_J \sim 2 \times M_{\text{BE}}$.

5.3.2. Accretion physics

In the early universe, protostellar accretion rates were likely much larger than today, due to the higher temperatures in the star forming clouds, which in turn is a consequence of the limited ability of the primordial gas to cool below the $\sim 200 \text{ K}$ accessible to H_2 -cooling. This argument would still be valid, even if a more efficient cooling agent, such as the deuterated hydrogen molecule (HD) or metal species, were able to tie the gas temperature to the floor set by the cosmic microwave background (CMB). Minimum temperatures in star forming clouds would thus remain higher than the canonical value in present-day molecular clouds (MCs) of $\sim 10 \text{ K}$, as long as $z \gtrsim 3$: $T_{\text{min}} \simeq T_{\text{CMB}} \gtrsim 11 \text{ K} (1+z)/4$. A useful estimate for the protostellar

accretion rate can be derived by assuming that a Jeans-mass worth of gas collapses on its free-fall time scale (see Ref. [36]):

$$\dot{M}_{\text{acc}} \simeq \frac{M_{\text{J}}}{t_{\text{ff}}} \simeq \frac{c_s^3}{G} \propto T^{3/2}. \quad (5.14)$$

Typical accretion rates are therefore higher by two orders of magnitude in primordial star forming regions, compared to Galactic ones (ratio $\propto (300/10)^{3/2}$). Initially, infall in the Jeans-unstable parent cloud proceeds in a predominantly spherical fashion, leading to the build-up of a hydrostatic core in the center of the minihalo, with typical mass $\sim 10^{-2} M_{\odot}$. Subsequent material, however, falls in with nonnegligible angular momentum, such that streamlines do not hit the central core right away. Instead, a rotationally supported disk is growing around the central core from the inside out. Crucially, those primordial protostellar disks are ubiquitously driven towards gravitational instability.

The basic physical argument, briefly, is as follows: Because of the very high accretion rates within a primordial pre-stellar core, $\dot{M} \lesssim 0.1 M_{\odot} \text{ yr}^{-1}$, the nearly Keplerian disk experiences rapid mass growth over a range of radii. There are strong gravitational torques present, acting to drive mass towards the center. Even at the maximum mass transport rates that can realistically be generated by such torques, however, the disk cannot process the incoming material quickly enough. Approximately, one can analyze this situation within the framework of a thin disk model, where the accretion rate is $\dot{M} \simeq 3\pi\nu_{\text{vis}}\Sigma$ (see Ref. [37]). Here, Σ is the mass per unit surface area, and the (kinematic) viscosity can dimensionally be written in terms of the disk sound speed and pressure-scale height, H_p , as $\nu_{\text{vis}} \simeq \alpha c_s H_p$. For gravitational torques, the Shakura–Sunyaev parameter is $\alpha \sim 0.1$ –1. Using typical values encountered in accretion disks around Pop III proto-stars, $\Sigma \sim 100 \text{ g cm}^{-2}$, $H_p \sim 100 \text{ AU} \sim 10^{15} \text{ cm}$, and $c_s \simeq 10^5 \text{ cm s}^{-1}$ (see Ref. [38]), we estimate $\dot{M} \lesssim 10^{-2} M_{\odot} \text{ yr}^{-1}$, well below the infall rates from the envelope.

This rate imbalance will drive the disk to a state where the Toomre Q -criterion for global gravitational stability, $Q = c_s \kappa / (\pi G \Sigma) > 1$, is violated. Here, κ is the epicyclic frequency, equal to the angular velocity (Ω) in a Keplerian disk. Thus, the disk is subject to global perturbations, such as spiral modes. To enable fragmentation, however, a second, stronger, criterion needs to be considered. This is the Gammie criterion, stating that for a density perturbation to survive the disruptive effect of disk shear, thus enabling successful fragmentation, the cooling time scale has to be shorter than the orbital one: $t_{\text{cool}} < 3\Omega^{-1}$. Simulations have shown that disk temperatures remain close to $T \simeq 2,000 \text{ K}$, even at densities high enough for opacity effects to become important. There is an effective thermostat provided by the collisional dissociation of molecular hydrogen, which absorbs 4.48 eV per dissociation event. This is somewhat of a “knife-edge” effect however. If the disk were just a bit hotter, resulting from an internal or external heating source, it may be possible to stabilize the disk accretion mode. Including the luminosity generated

by, possibly highly time-variable, gas accretion onto the protostar(s) does somewhat delay fragmentation, but cannot suppress it completely. This result, however, does only pertain to the early evolution, where photoionization has not yet become important. The behavior of the Pop III disks follows the same trends, in terms of fragmentation and stability, that govern protostellar disks in general (for a review, see Ref. [39]).

The likely outcome of this disk fragmentation mode is a group, or small cluster, of stellar multiples, spanning a wide range in mass, as described by the IMF, a topic to which we turn next.

5.3.3. Initial mass function

The stellar IMF is a complicated function of mass, but it is often convenient to simply write it as a power law, valid for a given mass range. Specifically, one considers the number of stars per unit mass:

$$\frac{dN}{dM} \propto M^{-x}, \quad (5.15)$$

where the present-day IMF is characterized by the famous Salpeter slope of $x = 2.35$. To understand what the *typical* outcome of the star-formation process is, one can ask: *Where does most of the available mass go?* Or, put differently: What is the average stellar mass? This can be calculated as follows:

$$\bar{M} = \frac{\int_{M_{\text{low}}}^{M_{\text{up}}} M \frac{dN}{dM} dM}{\int_{M_{\text{low}}}^{M_{\text{up}}} \frac{dN}{dM} dM} = \frac{1-x}{2-x} \frac{M_{\text{up}}^{2-x} - M_{\text{low}}^{2-x}}{M_{\text{up}}^{1-x} - M_{\text{low}}^{1-x}} \sim 3.8 \times M_{\text{low}}, \quad (5.16)$$

where in the last relation, we have used the Salpeter value for x , and M_{low} and M_{up} are the lower and upper mass limits, respectively. In general, one can neglect all terms involving M_{up} above, as long as $x > 2$. This means that a Salpeter-like IMF is dominated by the lower-mass limit. For Population I (present-day) stars, one often takes $M_{\text{low}} \simeq 0.1M_{\odot}$ and $M_{\text{up}} \simeq 100M_{\odot}$, such that $\bar{M} \sim 0.5M_{\odot}$, whereas for Pop III, current theory postulates a characteristic (typical) mass of $\bar{M} \sim 4M_{\text{low}} \sim \text{a few} \times 10M_{\odot}$, assuming that the Pop III IMF were to exhibit a slope similar to Salpeter. The latter assumption is not at all proven and just serves as a zeroth-order guess.

5.4. First galaxy assembly

5.4.1. Virialization and gas collapse

With the emergence of the first galaxies, we witness the onset of supersonic turbulence, which is expected to have important consequences for star formation (reviewed in Refs. [33, 40]). To explore this, we estimate the Reynolds and Mach

numbers as follows. The Reynolds number measures the relative importance of inertia and viscous forces:

$$Re = \frac{\text{inertial acceleration}}{\text{viscous acceleration}} \simeq \frac{\frac{V}{T}}{\nu \frac{V}{L^2}} \simeq \frac{VL}{\nu}, \quad (5.17)$$

where V , L , $T = L/V$ are characteristic velocity, length, and time scales, respectively. For the first galaxies, we can estimate: $V \sim v_{\text{vir}} \sim 10 \text{ km s}^{-1}$, $L \sim R_{\text{vir}} \sim 1 \text{ kpc}$, and $\nu \sim \lambda_{\text{mfp}} c_s \sim 10^{18} \text{ cm}^2 \text{ s}^{-1}$. For the last estimate, we have assumed $\lambda_{\text{mfp}} = 1/(n\sigma_{\text{coll}}) \sim 10^{13} \text{ cm}$, if the number density is typically $n \sim 10^3 \text{ cm}^{-3}$, and we consider collisions between neutral hydrogen atoms ($\sigma_{\text{coll}} \sim 10^{-16} \text{ cm}^2$). For the typical particle velocity, we assume the sound-speed of H_2 -cooled gas ($c_s \sim 1 \text{ km s}^{-1}$). The Reynolds number in the center of the first galaxies is therefore $Re \sim 10^9$, indicating a highly turbulent situation. The Mach number is $Ma \sim V/c_s \sim v_{\text{vir}}/c_s \sim 10$, indicating supersonic flows.

Supersonic turbulence generates density fluctuations in the ISM. Statistically, these can be described with a log-normal probability density function (PDF):

$$f(x)dx = \frac{1}{\sqrt{2\pi\sigma_x^2}} \exp\left[-\frac{(x - \mu_x)^2}{2\sigma_x^2}\right] dx, \quad (5.18)$$

where $x \equiv \ln(\rho/\bar{\rho})$, and μ_x and σ_x^2 are the mean and dispersion of the distribution, respectively. The latter two are connected: $\mu_x = -\sigma_x^2/2$. This relation can easily be derived by interpreting the PDF above as a distribution (of x) by volume. One then has for the volume-averaged density: $\bar{\rho} = \int \rho f(x)dx = \bar{\rho} \int e^x f(x)dx$, which yields the desired result. Numerical simulations have shown that the dispersion of the density PDF is connected to the Mach number of the flow: $\sigma_x^2 \simeq \ln(1 + 0.25Ma^2)$. Inside the first galaxies, one finds values close to $\sigma_x \simeq 1$. Similar to the well-studied case of isothermal, supersonic turbulence (e.g., Ref. [42]), the central gas in the first galaxies exhibits the imprint of self-gravity: a power-law tail toward the highest densities, on top of the log-normal PDF at lower densities, which is generated by purely hydrodynamical effects (see Fig. 5.2).

A useful way to characterize turbulence is by way of velocity structure functions, in particular the second-order function, $S_2 \propto \ell^{\zeta(2)}$. Here, ℓ is the distance over which the velocity differences are evaluated, and $\zeta(2) \simeq 1.04$, as determined in simulations, over the range $\sim 100\text{--}500 \text{ pc}$. One then finds a velocity-size relation, $S_2^{1/2} \propto \ell^{0.52}$, which is very similar to the ‘‘Larson-law’’ velocity-size relation for present-day MCs (see Ref. [43]). The huge Reynolds number of the underlying turbulence implies a very large dynamic range between the feeding scale, roughly the virial radius of an atomic cooling halo, $R_{\text{vir}} \sim 1 \text{ kpc}$, and the viscous dissipation scale. Even the most highly resolved simulations to date, employing some form of adaptive spatial refinement, will, therefore, not be able to fully capture the turbulent flows encountered. First attempts have been made to incorporate such unresolved turbulence with subgrid-scale (SGS) modeling, properly matched onto the resolved large-eddy simulation. It is not yet clear how robust such SGS modeling is and

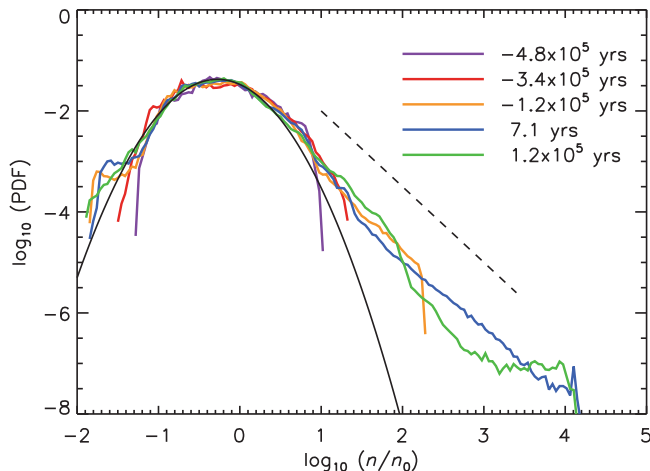


Fig. 5.2. Density fluctuations in the center of the first galaxies. The presence of supersonic turbulence is manifested in the characteristic log-normal probability distribution. At late times, self-gravity imprints a power-law extension toward high densities. It is possible that the turbulently structured gas will give rise to a high-mass slope in the stellar IMF, similar to the present-day Salpeter one. Adapted from Ref. [41].

how appropriate the calibrations used. Overall, these are still early days in the study of the coupled gravito-turbulent star formation process in the high-redshift universe, but it is likely that we will see rapid progress. A prime challenge is to work out the character of clustered star formation in the first galaxies, which must carry the imprint of the supersonic turbulence available inside of them. Advances in supercomputing power are getting us to the verge of simulating the formation of such chemically primitive stellar systems, in a completely *ab initio* fashion, from cosmological initial conditions to protostellar scales. We will now take a look at how such cosmological star formation calculations might turn out.

5.4.2. Star formation inside the first galaxies

The occurrence of Pop III SNe leads to the rapid, initial enrichment of the pristine IGM with a bedrock metallicity of $Z_{\min} \sim 10^{-3} - 10^{-2} Z_{\odot}$, at least locally in the biased regions of primordial star formation. Such levels of enrichment are well in excess of what has been termed “critical metallicity”, $Z_{\text{crit}} \sim 10^{-5} - 10^{-3.5} Z_{\odot}$, which is the minimum metallicity required to enable the formation of predominantly low-mass Pop II stars. Thus, the second generation of star formation will occur in already metal-enriched clouds, and the question is where this can take place. Theory suggests that conditions for recollapse are met in atomic cooling halos. Recall that these are DM systems with a total mass of $M \sim 10^8 M_{\odot}$, virializing at $z \sim 10 - 15$, and exhibiting virial temperatures of $T_{\text{vir}} \sim 10^4$ K.

During the early stage of collapse into an atomic cooling halo, the gas cools via fine-structure lines of O I, as well as C I and C II. For super-critical abundances

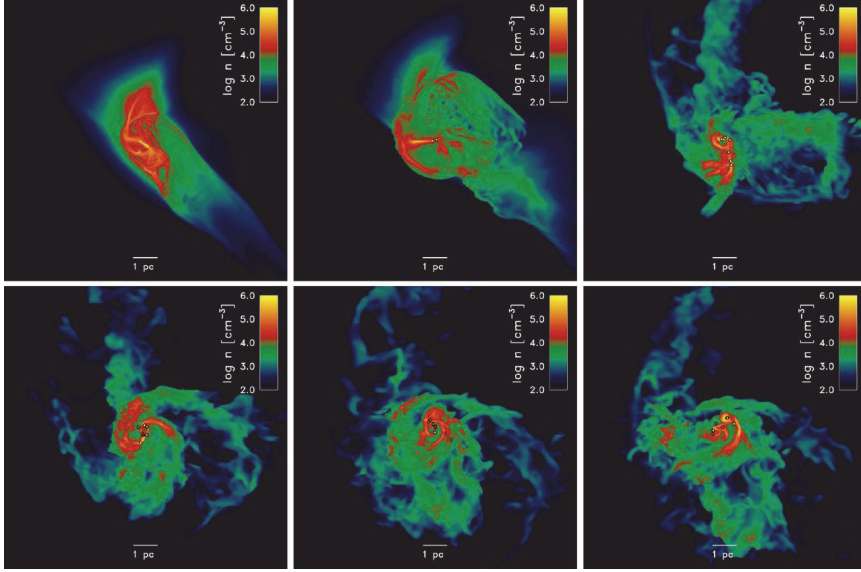


Fig. 5.3. Formation of Pop II stars inside the first galaxies. Shown are gas density projections, following the collapse and fragmentation in the center of the emerging galaxy, in a time series (from top-left to bottom-right) separated by 0.8 Myr. The gas is enriched to $10^{-2}Z_{\odot}$ from a previous generation of Pop III SNe. The open circles mark the location of sink particles, physically corresponding to pre-stellar clumps. These clumps give rise to clusters of Pop II stars. Adapted from Ref. [44].

($Z > Z_{\text{crit}}$), the gas is cooled to the temperature of the CMB, $T_{\text{CMB}} \simeq 50 \text{ K}$ at these redshifts. Infall velocities, on the other hand, are of the order $v_{\text{infall}} \simeq \sqrt{k_{\text{B}}T_{\text{vir}}/m_{\text{H}}} \simeq 10 \text{ km s}^{-1}$, which is larger than the sound speed $c_{\text{s}} \simeq \sqrt{k_{\text{B}}T_{\text{CMB}}/m_{\text{H}}} < 1 \text{ km s}^{-1}$. As we have seen above, the environment for the formation of the second generation of (Pop II) stars is thus supersonically turbulent, similar to the conditions in present-day MCs, but significantly different from the situation in the minihalos, where the first (Pop III) stars form. In the latter case, gas flows are subsonic, or at most transonic. Simulations of second-generation star formation indeed demonstrate the organization of the gas into a transient system of intersecting sheets and filaments, akin to the familiar picture in nearby MCs (see Fig. 5.3). Similar to the present-day case, star formation in the first galaxies is thus characterized by (i) low overall efficiencies and (ii) a power-law IMF, reflecting the self-similar nature of supersonic turbulence. The lesson here is that a near-universal IMF may already be in place very early in cosmic history, just one step after the first, somewhat singular, Pop III episode.

5.5. First BHs

Observations have shown that luminous quasars already existed at $z \gtrsim 6$ (see, e.g., [45, 46]). These sources were powered by the accretion of gas onto supermassive

black holes (SMBHs), with inferred BH masses of $\sim 10^9 M_\odot$. The existence of such supermassive objects early in cosmic history poses a challenge to our models of structure formation, related to the time scales involved in their assembly. Various scenarios for SMBH formation have been suggested (for a recent review, see Ref. [47]), including the growth from a Pop III stellar-mass seed BH by gas accretion and/or mergers with other stellar mass BHs. It turns out that there is a nontrivial obstacle to this formation path, provided by feedback from the first stars in the galaxies hosting the BHs. This feedback may impede gas accretion and thus delay BH growth for a sizable fraction of the local Hubble time, typically $\Delta t_{\text{delay}} \sim 100$ Myr. To see why this early “bottleneck” in the accretion process is problematic for the assembly of a high- z SMBH, it is instructive to consider the physics of Eddington-limited accretion.

Assuming that a BH is fed at a rate $\dot{M}_{\text{BH}}$, the release of gravitational potential energy from the infalling gas gives rise to a luminosity that can be parameterized as $L = \eta \dot{M}_{\text{BH}} c^2$, where $\eta \simeq 0.1 - 0.4$ is the radiative efficiency. Here, the larger efficiency corresponds to the accretion onto a maximally rotating Kerr BH. The photons thus produced by the accretion propagate outwards through the infalling envelope. In doing so, they may interact with the (mostly) ionized hydrogen gas through Thomson scattering on the free electrons, which in turn creates an outward-directed radiation pressure component. If we balance this pressure with the inward-directed force of gravity, we arrive at the well-known Eddington limit for the maximum luminosity that can be maintained by a radiatively efficient accretion flow

$$L_{\text{Edd}} = \frac{4\pi G m_{\text{H}} c M_{\text{BH}}}{\sigma_{\text{T}}} \simeq 3 \times 10^4 L_\odot \left(\frac{M_{\text{BH}}}{M_\odot} \right), \quad (5.19)$$

where σ_{T} is the Thomson cross-section. One can then ask: *How long does it take to radiate away the entire rest energy of an object at the Eddington rate?* This gives rise to the Salpeter time scale

$$t_{\text{Sal}} = \frac{M_{\text{BH}} c^2}{L_{\text{Edd}}} = \frac{c \sigma_{\text{T}}}{4\pi G m_{\text{H}}} \simeq 450 \text{ Myr}. \quad (5.20)$$

Combining these equations, and assuming that the source radiates at the Eddington rate, $L \simeq L_{\text{Edd}}$, we can obtain the BH’s history of mass growth

$$M_{\text{BH}}(t) = M_{\text{BH},0} \exp \left[\frac{1 - \eta}{\eta} \frac{t - t_0}{t_{\text{Sal}}} \right], \quad (5.21)$$

where t_0 is the time when the seed BH of mass $M_{\text{BH},0}$ begins to accrete. If we assume a radiative efficiency of $\eta \simeq 0.1$, and a stellar Pop III BH remnant, at the upper end of what is plausible, of $M_{\text{BH},0} \simeq 100 M_\odot$, we find that the BH can grow to $\sim 10^6 M_\odot$ in about 500 Myr. Simulations have shown that once million-solar mass holes have been assembled by $z \sim 10$, any feedback is unable to inhibit further

growth to reach the billion-solar-mass scale at $z \simeq 6 - 7$, required by the quasar observations (see Ref. [48]). Indeed, the critical phase, where stellar feedback may disruptively interfere, concerns the early growth from seed BH to $\sim 10^6 M_\odot$ ones. Now, our argument above seems to indicate that the growth time scale for a stellar seed is of the same order as the Hubble time at redshift $z \sim 10$, indicating that stellar-mass seeds may be able to successfully initiate SMBH assembly. However, as shown by recent simulations, early growth of Pop III stellar seeds is delayed by Δt_{delay} , creating a serious impasse on the available time to reach SMBH scales within ~ 0.5 Gyr.

This is why theorists have proposed the so-called direct collapse model for early SMBH formation (see Ref. [49]). The basic idea is to consider the collapse of metal-free gas into an atomic cooling halo with virial temperatures $T_{\text{vir}} \gtrsim 10^4$ K (see Section 5.2.2 above). In the direct collapse scenario, high temperatures are reached in halos where cooling by molecular hydrogen and metal lines to below $\simeq 10^4$ K has been suppressed, which implies that the only coolant acting on the gas is atomic hydrogen (see Ref. [18]). In the case of molecular hydrogen, which naturally forms at the center of the halo, its photodissociation can be achieved by an external soft ultraviolet (UV) background in the LW bands. Previous studies have found that this leads to a nearly isothermal collapse at $T \simeq T_{\text{vir}} \simeq 10^4$ K due to initially Lyman- α cooling, and subsequently H^- bound-free and free-free emission, when higher densities are reached. High-resolution simulations have shown that, as the gas collapses and reaches densities of $\simeq 10^{17} \text{ cm}^{-3}$, it becomes optically thick to H^- radiation, and a massive protostar with accretion rate $\simeq 1 M_\odot \text{ yr}^{-1}$ forms at the center of the halo. Due to this high accretion rate, the central object can easily become a supermassive star of $\simeq 10^5 - 10^6 M_\odot$ within a million years, which later might collapse into a SMBH due to relativistic instabilities. Thus, the direct-collapse model posits “collapse without fragmentation”, the latter, if present, would act to impede the SMBH assembly through stellar feedback. Once such a seed with $M_{\text{BH},0} \simeq 10^6 M_\odot$ is in place, subsequent growth will be efficient, in extreme cases accounting for the most luminous quasars detected at $z \gtrsim 6$.

A final requirement is that only a small fraction of all halos needs to experience runaway BH growth to reach the observed space density of SMBHs at $z \gtrsim 6$. Such limits may naturally be imposed by the requirement that the external LW radiation field has to be unusually strong, a few order of magnitudes larger than the cosmic mean value at those redshifts. This is often discussed in terms of a “critical” LW radiation intensity, $J_{\text{LW,crit}}$, which in units of the canonical high- z value of $10^{-21} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1} \text{ sr}^{-1}$, is of order $J_{\text{LW,crit}} \simeq 10^{-4} - 10^{-3}$. By way of comparison, the intensity to achieve reionization, by slightly more energetic photons in the far UV, is of order $J_{\text{FUV, reion}} \simeq 1$, in the same units. Another mechanism of self-regulation may have been the X-ray emission from accreting BHs, whose penetrating photoionization heating could have suppressed the collapse of gas into low mass halos, even long before reionization.

5.6. Observing the first galaxies

It is useful to recall the derivations of some of the key quantities in observational cosmology, specifically luminosity and angular-diameter distance, as well as the observed flux. It is also useful to assemble estimates for their typical values as encountered in the first galaxies. Further details are given in the monographs mentioned above. In addition, a comprehensive survey of high-redshift galaxy observations, including a description of the key methods and tools, is given in Ref. [50].

5.6.1. Cosmological distances

In analogy to the usual inverse-square law, the luminosity distance, d_L , is defined via

$$f_{\text{obs}} = \frac{\Delta E_{\text{obs}}}{\Delta t_{\text{obs}} \Delta A_{\text{obs}}} = \frac{L_{\text{em}}}{4\pi d_L^2}. \quad (5.22)$$

Here and in the following we refer to quantities that are measured at $z = 0$ with the subscript “obs” and with “em” to source-frame quantities (emitted at a given redshift z). Note that $\Delta E_{\text{obs}} = \Delta E_{\text{em}}/(1+z)$, and $\Delta t_{\text{obs}} = \Delta t_{\text{em}}(1+z)$ relate small differences in energy and time in the two frames. To evaluate ΔA_{obs} , carry out the following thought experiment: Imagine that you could somehow “step outside” our universe, looking down at the scene from some (higher-dimensional) bird’s-eye perspective. Such a perspective, which of course is completely inaccessible in practice, would allow you to measure distances, *as they would appear today*. Or, put differently, you somehow managed to stop the expansion of the universe, keep everything frozen at $z = 0$, and go about measuring the distance, with some appropriate measuring rod, from the observer (the telescope) to where the source would be located today. Recall that the source was much closer when it emitted the photon that we receive today, but has hence receded due to cosmic expansion. This source–observer distance, $r(z)$, is called *comoving distance* or *proper distance*. Although it cannot be directly measured, but instead can only be calculated by assuming a theoretical model of the universe, this concept is nevertheless extremely useful in cosmology. Assuming a point source at a given redshift z , we can now write the (proper) size of the spherical surface over which the photons have been spread as $\Delta A_{\text{obs}} = 4\pi r^2(z)$.

To calculate the comoving distance, consider the Robertson–Walker (RW) metric (see Chapter 1):

$$ds^2 = c^2 dt^2 - a^2 dr^2, \quad (5.23)$$

where we have assumed a spatially flat universe, and ds is the (invariant) space–time interval. Since they travel along null geodesics ($ds = 0$), one has for photons, $dr = c dt/a$ (recall $a = 1/(1+z)$). The RW metric describes any homogeneous,

isotropic, and expanding universe. To fully specify the background cosmological model, we also need the Friedmann equation, governing $\dot{a}$. The latter can in turn be derived from the Einstein field equations of general relativity (see Ref. [19]), yielding

$$\left(\frac{\dot{a}}{a}\right) = H(z) = H_0 \sqrt{\Omega_m(1+z)^3 + \Omega_\Lambda}, \quad (5.24)$$

where H_0 , Ω_m , and Ω_Λ are the Hubble constant, the density parameter for matter, and that for dark energy, respectively, as measured to very high precision by *WMAP* and *Planck* (see Ref. [32]). In this expression, we again assume a spatially flat universe (zero curvature). We can easily carry out the integration along the photon-geodesic:

$$r(z) = c \int_0^z (1+z') \left| \frac{dt}{dz'} \right| dz' = \frac{c}{H_0} \int_0^z \frac{dz'}{\sqrt{\Omega_m(1+z')^3 + \Omega_\Lambda}}, \quad (5.25)$$

where we use the Friedmann equation in the last step.

We have now all the ingredients in hand to find an expression for the luminosity distance:

$$f_{\text{obs}} = \frac{1}{4\pi(1+z)^2 r^2} \frac{\Delta E_{\text{em}}}{\Delta t_{\text{em}}} = \frac{L_{\text{em}}}{4\pi r^2 (1+z)^2}. \quad (5.26)$$

Comparing with the definition above, we finally have $d_L(z) = (1+z)r(z)$. It is useful to memorize the ballpark number for a source at $z \simeq 10$, appropriate for the first galaxies: $d_L(z) \sim 10^2$ Gpc.

Next, let us derive the analogous expression for *angular-diameter distance*, d_A , where we again start with a definition that follows basic, geometrical intuition. If a source at z , having a true (proper) transverse size of D , is observed to have an apparent angular size of Θ , we define $\Theta = D/d_A$. Let us again assume our bird's eye perspective as before. How would the source appear at the present-day ($z = 0$) if it had just been coasting along with the expanding universe since the time that the photons, reaching us now, were originally emitted? The situation can be described with a virtual triangle, where

$$\Theta = \frac{D(1+z)}{r(z)} = \frac{D}{d_A}, \quad (5.27)$$

giving us our result: $d_A = r(z)/(1+z)$. Note that the two fundamental distances of observational cosmology are connected: $d_L = d_A(1+z)^2$, such that it suffices to remember only one. For a first galaxy, where $D \sim 1$ kpc, one finds: $\Theta \sim D/d_A \sim 1 \text{ kpc}/1 \text{ Gpc} \sim 10^{-6} \sim 0.2''$. The near-IR camera on-board the *JWST* (NIRCam) should thus be able to marginally resolve these sources.

5.6.2. Observed fluxes

To estimate how bright a first galaxy is likely to be, we need to consider the observed specific flux (flux per unit frequency):

$$f_{\nu,\text{obs}} = \frac{\Delta E_{\text{obs}}}{\Delta t_{\text{obs}} \Delta A_{\text{obs}} \Delta \nu_{\text{obs}}} = \frac{\Delta E_{\text{em}} / (1+z)}{4\pi r^2 \Delta t_{\text{em}} \Delta \nu_{\text{em}}} \simeq (1+z) \frac{L_{\nu,\text{em}}}{4\pi d_L^2}. \quad (5.28)$$

To arrive at a zeroth-order guess, we assume that the total stellar mass involved in the starburst at the center of a first galaxy is $M_* \sim 10^5 M_\odot$. If we further assume that we are dealing with a top-heavy Pop III burst, the stellar radiation will be characterized by $T_{\text{eff}} \sim 10^5$ K, corresponding to a peak frequency of $\nu_{\text{max}} \sim 10^{16}$ Hz, and a total luminosity close to the Eddington luminosity: $L \sim L_{\text{EDD}} \sim 10^{43}$ erg s $^{-1}$. The emitted specific luminosity is thus $L_{\nu,\text{em}} \sim L_{\text{EDD}} / \nu_{\text{max}} \sim 10^{27}$ erg s $^{-1}$ Hz $^{-1}$. The observed (specific) flux for a first galaxy at $z \sim 10$ is then

$$f_{\nu,\text{obs}} \sim 10^{-32} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1} = 1 \text{ nJy}. \quad (5.29)$$

The nJy is indeed the typical brightness level that the *JWST* is designed to image with NIRCам, thus reiterating the point that with this next-generation facility, we will get the first galaxies within reach of deep-field exposures.

5.6.3. Local probes

How can the simulation results be tested, other than with *in situ* observations at high redshifts, where sources are dim, and signal-to-noise ratios will typically be poor? There is an ideally complementary approach for the second stage of star formation out of already metal-enriched material, given that Pop II star formation will leave long-lived stellar systems behind. Those “fossils” can be directly probed in the Local Group, in the halo of the Milky Way, and in surrounding dwarf galaxies, in the stellar archaeological, or near-field cosmological approach (see Refs. [27, 28]). As an example, the measured IMF in dwarf galaxies can be compared with simulation results (see Section 5.4.2). There are hints for a flattening of the IMF power-law slope in the Small Magellanic Cloud (SMC) and in some UFDs, such as Leo IV (see Ref. [51]). Simulations are just reaching the dynamic range to study the formation of Pop II stellar clusters in sufficient detail to derive predicted IMFs, to be compared with the observations (e.g., see Ref. [44]). These are early days for such “cosmological star cluster simulations”. Prospects for the future, however, are good to robustly work out the connection between the linear physics of the cosmological initial conditions and the nonlinear consequences in the formation of stars and their clusters. An increasingly key role in stellar archaeology will likely belong to the local UFDs because they provide ideal laboratories to test the *ab initio* simulations of first galaxy formation (e.g., Ref. [52]). A complete census of their entire stellar content may be achievable in the imminent era of the extremely large telescopes, to

be compared with theoretical predictions for these “maximally primitive” systems, in terms of their chemical, stellar, and structural assembly histories.

5.7. New horizons

The next decade will be very exciting as we are opening up multiple windows into the cosmic dark ages. We will finally be able to close the remaining gap in the long quest to reconstruct the entire history of the universe, which began with the pioneers of cosmology in the 1920s. There will be many opportunities to make important discoveries, e.g., in directly detecting the first sources of light and in working out a well-tested theoretical framework for star and galaxy formation at the dawn of time. Very likely, serendipity will play a crucial role. It is thus a good idea to equip oneself with a comprehensive set of tools, such as the basic physics covered in this volume. It is also clear that ever more sophisticated numerical simulations will continue to provide heuristic guidance for our journey into the unknown. Thus, to a young theorist at the beginning of her/his career, no better advice can be given than to acquire numerical mastery, combined with a firm grip on the equally important emerging field of “Big Data”, given the extremely data-rich character of upcoming observations.

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Chapter 6

Galaxy Formation and Evolution

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In this chapter, we discuss basic physics of galaxy formation and evolution in cosmological hydrodynamic simulations. First, we describe some of the basic physical processes for galaxy formation, such as radiative cooling and heating of gas, star formation, and supernova (SN) feedback models. Second, we discuss basic output of simulations: star formation rate density (SFRD), galaxy stellar and luminosity functions as a function of time. Feedback processes by supernovae and supermassive black holes are considered to be the key for galaxy evolution, and various implementations have been attempted in cosmological hydrodynamic simulations over the past two decades.

6.1. Cosmological structure formation and galaxies

Within the framework of current best-fit Λ CDM model, structure formation in the Universe is driven by the gravity of dark matter (DM). As we reviewed in Chapter 1, we know that matter fluctuation at the time of recombination was on the order of $\delta \equiv (\rho - \bar{\rho})/\bar{\rho} \sim 10^{-5}$ from the measurement of CMB temperature anisotropy. It is believed that these fluctuations originated from the quantum fluctuations in the early Universe, and they later grew into the structures that we see today via gravitational instability. DM fluctuations grew first and created the large-scale structure such as filaments and voids. This initial phase of structure formation can be described by the linear perturbation theory, and it has been demonstrated well by the N -body simulations as discussed in Chapter 2. Underdense regions between

the filaments are called voids, and those regions evolve as if they were a low-density universe with $\Omega_M < 1$ [1].

As the DM pulled each other and the fluctuations grew, DM halos of different masses and sizes formed. The early phase of DM halo formation can be treated by the spherical collapse model [2] which we discuss in Section 6.2. In a CDM universe, lower mass halos formed first, and they later merged into more massive halos. Perturbations of baryonic gas lagged behind that of DM, and later caught up and fell into the potential well of DM halos.

As the gas falls into DM halos, it heats up due to compression and virial shock heating. At the same time, infalling gas can cool by emitting photons, i.e., radiative cooling, which is discussed in Section 6.4 as well as in Chapters 3 and 5. As the gas virializes, it experiences virial shock heating, and the temperature rises to the virial temperature of the DM halo:

$$T_{\text{vir}} = \frac{\mu m_p}{2k_B} V_c^2 \simeq 3.6 \times 10^5 \text{ K} \left(\frac{V_c}{100 \text{ km s}^{-1}} \right)^2, \quad (6.1)$$

where V_c is the circular velocity of DM halo, μ is the mean molecular weight of gas, m_p is the proton mass, and k_B is the Boltzmann constant.

6.2. Spherical collapse model for DM halo formation

The spherical collapse model is a very simple, yet very useful theoretical model that can bridge the gap between linear perturbation theory and nonlinear regime of halo collapse. In the standard spherical collapse model [2–4], a mass shell in an overdense region will first expand together with the Hubble expansion, reach a maximum radius, and then collapse when the gravitational pull overcomes the initial cosmological expansion.

Specifically, for a flat Λ CDM cosmology, the behavior of a spherical mass shell is described by the following equation of motion:

$$\frac{d^2 r}{dt^2} = -\frac{GM(< r)}{r^2} + \frac{\Lambda}{3} r, \quad (6.2)$$

where r is the physical radius from the center of the overdensity, G is the gravitational constant, $M(< r)$ is the enclosed mass within the shell, and Λ is the cosmological constant (or dark energy). On small scales ($\lesssim 1$ Mpc), generally the first term on the right-hand side is greater than the dark energy term, therefore the mass shell stalls due to inward gravity and then “turns around” at a radius “ r_{ta} ”. After a shell turns around, it decouples from the Hubble flow and then only feels the acceleration from dark energy. One can make a correspondence between Eq. (6.2) and general-relativistic Friedmann equation which we introduced in Chapter 1.

In Einstein–de Sitter universe ($\Omega_M = 1$, $\Omega_\Lambda = 0$), turnaround occurs when the average density within the sphere is $\simeq 5.6$ times the background density. A “virialized” halo has an average overdensity of $18\pi^2 = 178$ based on the collapse of a

spherical top-hat perturbation, a value that many authors round to 200 (see Ref. [5] for a generalization of this model to $\Omega_\Lambda > 0$).

The spherical collapse model also predicts the spherically averaged, radial density profiles resulting from the gravitational collapse of perturbations in an expanding universe [2, 3, 6, 7]. However, the spherical collapse model cannot be fully trusted once shell-crossing occurs because the mass enclosed within the shell is no longer constant. More in-depth study of physical properties of DM halos such as density profile and collapse redshift has to be performed with high-resolution N -body simulations, as discussed in Chapter 2 and by, e.g., Ref. [8].

6.3. DM halo mass function

The number density of DM halos as a function of mass and redshift can be computed by the Press–Schechter theory [9]. This function was derived from a simple but ingenious ansatz that the fraction of mass in the Universe that is included in collapsed halos with mass greater than M , $\mathcal{F}(> M)$, is roughly equal to the probability of $\delta_s > \delta_c$:

$$\mathcal{F}(> M) = 2\mathcal{P}(> \delta_c), \quad (6.3)$$

where δ_s is the smoothed overdensity, δ_c is the critical overdensity corresponding to the collapsed mass M , and a factor 2 on the right-hand side accounts for the fact that $\mathcal{P}(> \delta_c) \rightarrow 1/2$ when $M \rightarrow 0$, which implies that only half of mass in the universe is part of collapsed objects. If the matter fluctuation follows a Gaussian distribution,

$$P(\delta)d\delta = \frac{1}{\sqrt{2\pi\sigma_M^2}} \exp\left(-\frac{\delta^2}{2\sigma^2}\right) d\delta, \quad (6.4)$$

then

$$\mathcal{P}(> \delta_c) = \int_{\delta_c}^{\infty} P(\delta)d\delta = \text{erfc}\left[\frac{\delta_c}{\sqrt{2}\sigma_M}\right]. \quad (6.5)$$

Comoving number density of DM halos at redshift z within a mass range of $(M, M + dM)$ can be written as

$$n(M, z)dM = \sqrt{\frac{2}{\pi}} \frac{\bar{\rho}}{M} \frac{d\nu}{dM} \exp\left(-\frac{\nu^2}{2}\right) dM, \quad (6.6)$$

where $\nu \equiv \delta_c/[D(z)\sigma(M)]$, $\delta_c = 1.69$ is the critical overdensity for collapse, and $\sigma(M)$ is the variance of mass fluctuations as defined by Eq. (1.26) in Chapter 1. It is sometimes written as $n(M, z) \equiv dn/dM$. The growth factor is given by $D(z) = g(z)/[g(0)(1+z)]$, where an approximation for function $g(z)$ is given by, e.g., [10].

A nice summary of how to compute the halo mass function can be found in Ref. [11], which includes a description of the Sheth — Tormen mass function [12, 13] considering the ellipsoidal collapse of DM halos.

6.4. Radiative cooling of gas

Gas cools by radiating photons, and galaxies and stars cannot form in this Universe without radiative cooling. There are several channels for this process, for example, (i) collisional excitation of atoms, followed by de-excitation of an electron and emission of a photon, (ii) bremsstrahlung, and (iii) metal-line cooling.

Over the years, various cooling modules have been developed for cosmological hydrodynamic simulations (CHS). For example, various reaction rates have been summarized by Ref. [14], and examples of cooling functions are presented in Refs. [15–17]. Including the contributions of various metal lines is quite important for simulations of galaxy formation because metal-line cooling enhances the cooling rate significantly, as shown in Fig. 6.1. As structure formation proceeds in the

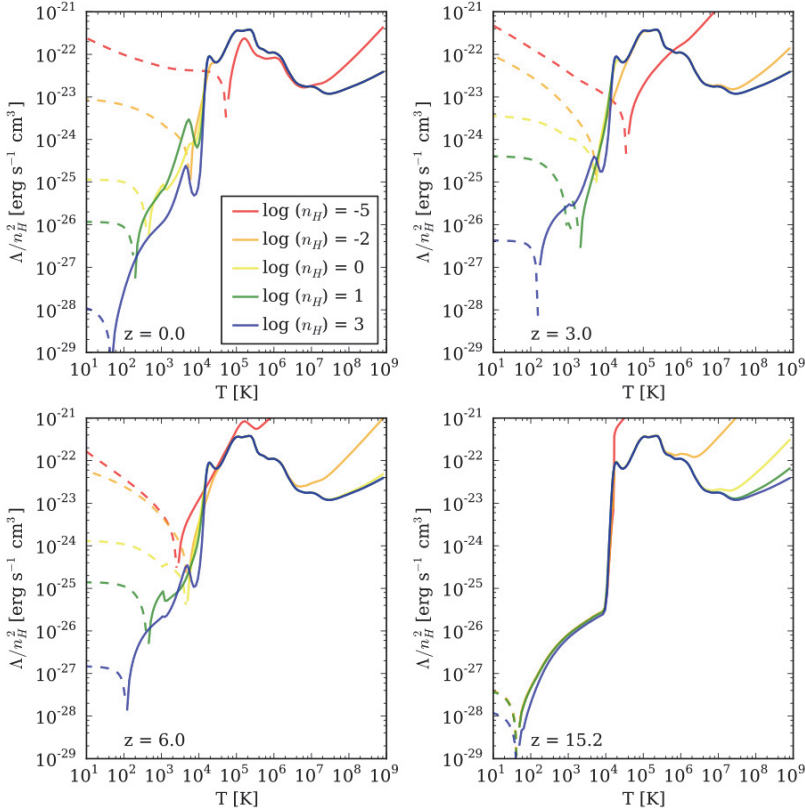


Fig. 6.1. Equilibrium cooling rates normalized by n_{H}^2 at redshifts $z = 0.0, 3.0, 6.0, 15.2$ from top-left to bottom-right panels, respectively. Both net cooling (solid line) and heating rates (dashed line) are shown for solar metallicity and hydrogen number densities of $n_{\text{H}} = 10^{-5}$ (red), 10^{-2} (orange), 1 (yellow), 10 (green), and 10^3 (blue) cm^{-3} . These rates were computed by the GRACKLE chemistry and cooling library using the nonequilibrium chemistry network of H, He, H_2 , and HD with a tabulated metal-cooling rates under the influence of UV background radiation from Ref. 22. Figure reproduced from Ref. 23 by permission of the AAS.

Universe, stars form in galaxies, and the gas in galaxies and intergalactic medium (IGM) are enriched by the metals ejected by supernova (SN) explosions from high redshift to the present time. Treating this chemical enrichment process together with star formation, SN feedback and gas recycling is crucial for subsequent star formation processes.

The cooling rate for a gas without metals have two distinct peaks just above 10^4 K from recombination of hydrogen (H) and helium (He), with an extended wing towards higher temperatures at $T \gtrsim 10^7$ K by bremsstrahlung with $\propto T^{1/2}$ dependence (see also Fig. 5.1). At temperatures below 10^4 K, the emission lines from H_2 molecules and forbidden lines of carbon (e.g., [CII] $158\ \mu\text{m}$ line), oxygen, etc. contribute at a much lower level, although they are quite important for the early structure formation at high redshift (see Chapters 4 and 5). For example, DM halos of $\sim 10^8 M_\odot$ with $T_{\text{vir}} \sim 10^4$ K form at $z \approx 10\text{--}15$, and star formation (such as the “first stars”) in lower mass halos ($\sim 10^6 M_\odot$) with primordial gas (i.e., without metals) has to rely on H_2 cooling at $T < 10^4$ K.

The metal-line cooling rate peaks at intermediate temperature range of $T \sim 10^{5.5}$ K, and the oxygen doublet lines in the far-UV (O VI $\lambda\lambda 1032, 1038\ \text{\AA}$) are the major coolant around this temperature [15]. These lines are observed in various environment, interstellar medium (ISM), circumgalactic medium (CGM) and IGM, and offer important clues for the “missing baryon problem” (e.g., [18]). The gas in the range of $T \sim 10^5\text{--}10^7$ K is called “Warm-Hot IGM” (“WHIM”), which is a large reservoir of baryons at low redshift [19, 20]. Often, collisional ionization equilibrium (CIE) is assumed in the calculation of these cooling rates, but one has to be careful as photoionization may strongly influence the cooling efficiency in this temperature range [21].

For diffuse IGM, heating from ultraviolet background (UVB) radiation is quite important, as the photoionization equilibrium is established between the heating rate from UVB and cooling rate [24]. Many UVB models have been developed [22, 25–27], and the consistency checks between the UVB model, mean photoionization rate measurement from $\text{Ly}\alpha$ forest, and the numerical simulation of IGM have proven to be quite useful probes of cosmic UVB and the thermal state of IGM. See Chapter 8 for more detailed discussions on $\text{Ly}\alpha$ forest using CHS.

Many cooling packages are now available in the astrophysical community with detailed treatments of chemical reaction network, e.g., GRACKLE chemistry and cooling library (see [23, 28, 29], <https://grackle.readthedocs.org/>), and KROME (see [30], <http://kromepackage.org/>). Here, we show example cooling curves in Fig. 6.1 from GRACKLE, which provides a nonequilibrium primordial chemistry network for atomic H and He [31, 32], H_2 and HD [33, 34], Compton cooling off the CMB, tabulated metal-cooling and photoheating rates from the photoionization code CLOUDY [35–37]. A look-up table for equilibrium cooling is also available in these cooling packages. Inverse of the cooling rate gives the cooling time, and one can compare it with the Hubble time to see which mass scales are able to cool and collapse to form galaxies within the Hubble time (see [38, 39]).

6.5. Star formation models in CHS

In CHS, we need to deal with enormous spatial scales from ~ 100 Mpc, where large-scale structure forms, to $\lesssim 100$ pc scales where molecular clouds and stars form. Since the physical processes of star formation (i.e., formation of proto-stars and proto-planetary disks) take place on $\sim$ AU scales, it is still impossible to treat the details of star formation concurrently with the formation of large-scale structure using current supercomputers. Therefore, we need to resort to subgrid (or sub-particle) models for star formation and feedback in CHS of galaxy formation, and attempt to capture the impact of sub-kpc scale physics onto larger scales.

One of the first subgrid models of star formation (SF) adopted the following criteria in an Eulerian simulation box of comoving $80 h^{-1}$ Mpc and 200^3 cells [40]:

$$\delta > \delta_{\text{SF}} \quad (\text{overdense}), \quad (6.7)$$

$$\nabla \cdot \mathbf{m}\mathbf{v} < 0 \quad (\text{converging gas flow}), \quad (6.8)$$

$$t_{\text{cool}} < t_{\text{dyn}} \quad (\text{cooling fast}), \quad (6.9)$$

$$m_b > m_J \quad (\text{Jeans unstable}), \quad (6.10)$$

where δ_{SF} is the SF threshold overdensity, t_{cool} is the cooling time, t_{dyn} is the dynamical time, m_b is the baryonic fluid element in the cell, and m_J is the Jeans mass. For a smoothed particle hydrodynamics (SPH) code, Ref. [41] adopted

$$\frac{h_i}{c_i} < \frac{1}{\sqrt{4\pi G \rho_i}}, \quad (6.11)$$

i.e., (sound crossing time) < (dynamical time), instead of Eq. (6.10), where h_i is the SPH smoothing length, c_i is the local sound speed, and ρ_i is the local gas density. These star formation criteria still form the basis of those that are used in modern simulations.

Once the fluid element satisfies above criteria, a collisionless star particle is generated according to

$$m_\star = m_b \Delta t / t_{\text{dyn}}, \quad (6.12)$$

and placed at the center of the cell with the same proper velocity as the gas in the cell [40]. In SPH codes, usually the expected star formation rate (SFR) is computed first for each SPH particle by

$$\dot{\rho}_\star = \epsilon_\star \frac{\rho_{\text{gas}}}{t_{\text{dyn}}}, \quad (6.13)$$

where $\rho_\star$ is the stellar mass density, $\epsilon_\star$ is the star formation efficiency, and ρ_{gas} is the gas density of an SPH particle. Then a star particle is spawned from the gas

particle stochastically in such a way that reproduces the above SFR when averaged over a long time. Different variations exist for the SFR calculation, for example,

$$\dot{\rho}_\star = (1 - \beta) \frac{\rho_c}{t_\star}, \quad (6.14)$$

where β is the gas recycling fraction, ρ_c is the cold gas density available for star formation, and $t_\star$ is the star formation time scale. Yepes *et al.* [42] and Springel and Hernquist [43, 44] developed multiphase ISM models to compute cold and hot gas densities, and adjusted the normalization of $t_\star = t_0(\rho/\rho_{\text{th}})^{-0.5}$ via t_0 to reproduce the observed Kennicutt–Schmidt law [45], which resulted in $t_0 \approx 1\text{--}2$ Gyr. It is often assumed that the star formation time scale is proportional to the local dynamical time, $t_\star \propto (G\rho)^{-0.5}$, which leads to $\dot{\rho}_\star \propto \rho^{1.5}$. The value of β is determined by the initial mass function (IMF) of stars and the choice of its mass range, with typical values of $\beta \approx 0.1$ (for a Salpeter IMF [46]) and 0.2 (for a Chabrier IMF [47]) as summarized in Refs. 48, 49. The gas is recycled into the ISM by SN explosions, therefore the value of β is closely linked to the feedback processes which will be discussed in the next section. Note that the overall gas recycling fraction for a simple stellar population (SSP) could increase to as high as ~ 0.45 at the age of 13.5 Gyr (see Fig. 2 of Ref. 48).

The produced star particles are treated thereafter as collisionless particles just like DM particles, therefore it will increase the computational cost at later times if you produce too many of them. To limit the total number of star particles and save computing time, the mass of star particles are often limited to only a certain fraction of gas particles in the case of SPH, such that one SPH particle turns into only a few star particles.

As the numerical resolution improves, the multiphase nature of ISM can be considered in more detail. Even when we do not have sufficient resolution to resolve below ~ 100 pc, we could implement a subgrid model that considers the molecular hydrogen (H_2) physics because star formation is strongly correlated with dense, cold molecular gas [50, 51]. In such multiphase ISM models, one can replace ρ_{gas} or ρ_c in Eqs. (6.13) and (6.14) to ρ_{H_2} as has been experimented by Refs. 52, 53, 54.

In the early simulations, the value of $\epsilon_\star$ was often taken to be in the range of $\epsilon_\star \approx 0.1\text{--}0.3$ [55, 56]. However, lower values of a few percent ($\epsilon_\star \sim 0.02$) began to be more favored later, based on the observational implications of slow star formation efficiency [57]. At the same time, there are some reports that the simulation results do not change very much at late times no matter which value of $\epsilon_\star$ you take, and some researchers have simply taken $\epsilon_\star = 1.0$ [58, 59], with the idea that star formation is self-regulated by feedback effects rather than the star formation law itself. Therefore, the resulting SFR density is more dependent on the feedback prescriptions rather than the exact value of $\epsilon_\star$.

One may argue that the value of $\epsilon_\star$ should be changed according to the resolution of the simulation because the detailed implementation of star formation and feedback would depend on it. If the simulation has sufficient resolution of $\ll 100$ pc

to resolve the formation and destruction of giant molecular clouds (GMCs), then one may follow more detailed feedback processes (e.g., radiative and stellar wind feedback) to treat the GMC lifetimes accurately. In this case, one expects that the observed low efficiency of star formation will be an “outcome” of the simulation rather than the input and therefore would want to change Eq. (6.13) to $\dot{\rho}_\star = \rho_{\text{mol}}/t_{\text{ff}}$, i.e., 100% efficiency per free-fall time with a high threshold density of $n_{\text{th}} \approx 100 \text{ cm}^{-3}$ [59, 60]. On the other hand, if the resolution is $>100 \text{ pc}$, then the GMC is unresolved and one would have to set the kpc-scale star formation efficiency of a few percent by hand with a lower threshold density of $n_{\text{th}} \approx 0.1 \text{ cm}^{-3}$ as is often the case for CHS with a large box size. This is still an area of ongoing research utilizing higher resolution zoom-in simulations, and we need to continue to perform CHS with larger box sizes as well as higher resolution zoom-in simulations and compare with various observations.

6.6. Overcooling problem, SN feedback, and galactic winds

In the early CHS, the thermal energy from supernovae (SNe) were simply deposited in the neighborhood of star forming regions. Naively, one expects that the gas becomes hot and expands as a hot bubble, thereby converting the thermal energy into the kinetic energy of ejecta. However, it was soon discovered that such conversion from thermal to kinetic energy was not taking place in the simulation; instead, the thermal energy was immediately radiated away because the energy was deposited into high-density regions. In other words, SN feedback was inefficient, gas was cooling too much, and stars were overproduced. This is known as the “*overcooling problem*” in CHS, and it stems from the fact that we do not have sufficient resolution in CHS to resolve the details of SN bubble expansion on small scales.

To remedy this problem, various methods have been proposed. One popular method is to introduce a kinetic feedback by hand, as we describe some examples below. Initially, SN energy is released in the form of radiation from radioactive decay, but a part of this energy will thermalize eventually and form a hot expanding bubble. The hot bubbles will percolate and form a “superbubble”, which eventually erupts from galactic disk and cause galactic winds (also called as “superwinds”). These galactic winds are observed in both local starburst galaxies such as M82 and high-redshift Lyman-break galaxies (e.g., [61, 62]). The energy balance between thermal and kinetic feedback is not well understood, but it is usually treated as input parameters of the SN feedback model.

In CHS, the star particles typically have masses greater than $10^4 M_\odot$ due to limited resolution, hence they are treated as SSP and tagged by various physical quantities such as formation time, stellar mass, and metallicity. Based on these quantities, one can follow the time evolution of SSP using a stellar population synthesis code and compute the expected number of SNe. For example, Type II SNe that would explode from progenitor stars with $M_\star > 8 M_\odot$ would correspond

to ~ 0.01 SNe per $1 M_\odot$ of stars [23]. Usually, it is assumed that $E_{\text{SN}} \sim 10^{51}$ erg per SN is injected into the ambient medium as a thermal energy, and about 30% of this energy could couple to the gas to cause galactic winds. In other words, the kinetic energy of galactic wind per $1 M_\odot$ of stars formed is

$$E_w \sim 10^{51} \times 0.3 \times 0.01 = 3 \times 10^{48} \text{ erg } M_\odot^{-1}. \quad (6.15)$$

For example, Ref. 56 adopted the following equations for galactic wind feedback:

$$\dot{E}_w = \epsilon_w \dot{M}_* c^2, \quad (6.16)$$

$$\dot{M}_w = \eta \dot{M}_*, \quad (6.17)$$

where $\epsilon_w = 3 \times 10^{-6}$ is taken for the energy efficiency of galactic wind, $\eta \approx 0.3$ is the mass-loading factor, c is the speed of light, and $\dot{M}_*$ is SFR. The kinetic feedback energy given in Eq. (6.15) corresponds to the efficiency of $\epsilon_w = (E_w / \dot{M}_* c^2) \sim 2 \times 10^{-6}$. Relating Eq. (6.16) to the wind velocity via $\dot{E}_w = \frac{1}{2} \dot{M}_w v_w^2$, above efficiencies imply that the wind velocity is

$$v_w \sim \left(\frac{\epsilon_w}{\eta} \right) c \sim 1500 \text{ km s}^{-1}, \quad (6.18)$$

but this may slow down to few hundred km/s when the ejecta has accumulated an amount of mass comparable to its initial mass [56]. The observed galactic wind velocity for Lyman-break galaxies at $z \sim 3$ is a few 100 km/s [63], therefore above efficiencies are chosen to be consistent with high- z galaxy observations. Cen *et al.* [56] injected E_w as a thermal energy into 27 local cells around the star particle, and others have also taken somewhat larger efficiencies of $\epsilon_w = 10^{-5}$ [64].

In the case of SPH simulations, one has to specify which particles receive the feedback energy. Some researchers simply adopt the smoothing kernel, or some compute the radius of an SN blast wave radius using Sedov–Taylor-like solutions [65–67] and distribute both thermal and/or kinetic energy to the gas particles inside this radius [68–71].

Observations indicate that the mass-loading factor is not constant, and it might depend on galaxy mass, SFR, or halo mass. The DEEP2 galaxy survey found $v_w \propto (\text{SFR})^{1/3}$ [72]. This can be understood roughly as $v_w \sim v_{\text{vir}} \sim M_h^{1/3} \sim (\text{SFR})^{1/3}$, i.e., the wind velocity has to be comparable to or greater than the virial velocity of the halo to escape, and the virial velocity is proportional to $M_h^{1/3}$. Crudely speaking, the SFR in each halo is roughly proportional to the total amount of baryons in the halo, which in turn can be expected to be proportional to the halo mass, although we know that the gas fraction has a significant scatter and lower than the cosmic mean ($\Omega_b / \Omega_{\text{DM}}$) owing to the feedback effects. Therefore, the above proportionality is a naive expectation that holds only for a limited mass range.

Theoretical arguments suggest two possible scalings for η [73]:

$$\eta \propto \begin{cases} \sigma^{-2} & (\text{Energy-driven wind}), \\ \sigma^{-1} & (\text{Momentum-driven wind}), \end{cases} \quad (6.19)$$

where σ is the velocity dispersion of stars in the galaxy, representing the potential well of the halo. For energy-driven wind, $\frac{1}{2}\dot{M}_w v_w^2 \propto E_{\text{SN}} \propto \text{SFR}$, and combining this with Eq. (6.17), one obtains Eq. (6.19). Momentum-driven wind considers the momentum input from the radiation of massive stars onto the ambient dust, which entrains gas to form stellar feedback from massive stars. Sometimes, this is called the “stellar feedback”. Since σ represents the depth of potential and it is also costly to compute the velocity dispersion in simulations, one often uses halo properties (virial mass, radius, velocity) instead of σ for implementing wind models, and it has been shown that introducing the momentum-driven wind produces better agreement with various galaxy statistics [74, 75]. One may try to utilize both types of winds in a single simulation depending on the environment; for example, the momentum-driven wind may dominate closer to the young massive stars and SNe in high-density regions where the UV radiation is stronger and pushes out the gas and dust more efficiently [75]. Ultimately, we would like to “predict” the dependence of η on galaxy stellar mass or halo mass using high-resolution simulations more physically, as was done by some recent zoom-in CHS [76].

6.7. Cosmic star formation rate density

The star formation model in CHS allows us to compute SFR per comoving volume, i.e., cosmic star formation rate density (SFRD). This is one of the most basic outputs (without any post-processing) obtained from *ab initio* hydrodynamic simulations (e.g., [48, 77–79]). The cosmic SFRD as a function of redshift is well known as the “Lilly–Madau diagram” after those who put the early observational data points on this diagram in a cosmological context [80, 81], and there have been vigorous observational efforts to add more data points at both low and high redshifts (e.g., [82–85] and references therein). Theorists simulate the cosmological evolution forward in time from high- z to low- z , whereas observers see the Universe in the opposite direction from the present time towards higher redshift.

The SFRD initially increases from $z \sim 20$ to $z \sim 6$ due to gravitational instability, following vigorous formation of DM halos in the early universe (Fig. 6.2, [43]). After experiencing its peak at an intermediate redshift range (somewhere between $z \approx 2$ – 6), the SFRD declines towards low redshift from $z \sim 1$ to the present time. This final decline of SFRD at low- z can be a combined effect of following multiple factors: (i) stalling growth rate of structures due to cosmic expansion; (ii) accelerating cosmic expansion due to dark energy is preventing active gas accretion onto DM halos at late times; (iii) feedback effects by SN and AGN are heating up the gas and preventing further star formation; (iv) consumption of gas due to past star formation histories.

In CHS, there are inevitable effects of box sizes and resolution on SFRD, and one has to be careful in interpreting the comparison between simulations and observations, as shown clearly in Fig. 6.2. For a given number of particles or cells that

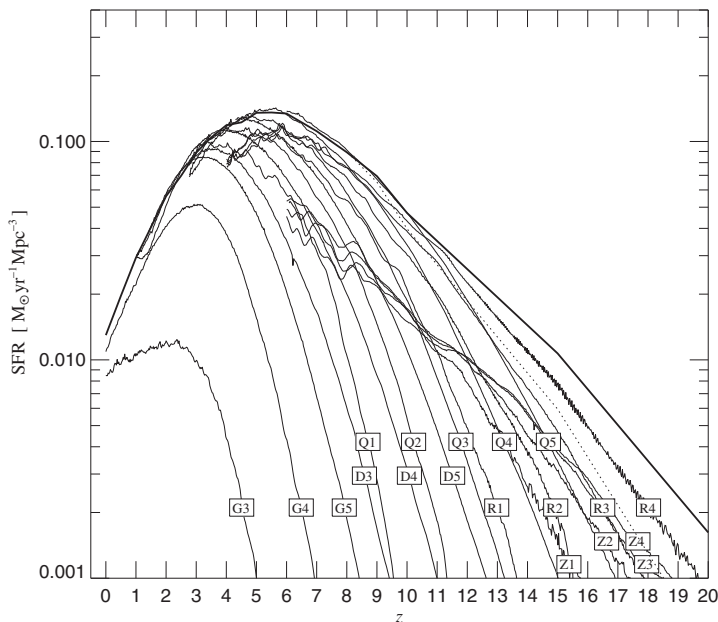


Fig. 6.2. Cosmic SFRD as a function of redshift from many CHS [43], showing the resolution and box-size effect. The alphabet indicates the simulation box size ($R = 3 h^{-1}$ Mpc, $Q = 10 h^{-1}$ Mpc, $D = 33.75 h^{-1}$ Mpc, $G = 100 h^{-1}$ Mpc), followed by a level number that indicates resolution (64^3 , 96^3 , 144^3 , 216^3 , 324^3 SPH particles for levels 1–5, respectively). The star formation starts earlier with a higher resolution as more low-mass halos are resolved at earlier times.

one uses (i.e., for a given computational resource), the resolution becomes better if you reduce your box size, and the star formation begins earlier as you resolve more low-mass halos at higher redshift. However, with a small box size, one cannot capture the collapse of long wavelength perturbations, and such a simulation becomes physically implausible at low redshift. Typically, with a simulation box size of comoving $10 h^{-1}$ Mpc, one would stop the simulation at $z \sim 2-3$. In Fig. 6.2, one can see that the simulations follow an upper locus before they deviate from it due to resolution effects, and Springel and Hernquist [43] provided an analytic formula for this locus based on an argument of halo growth and SFR distribution function. In Fig. 6.2, the peak of SFRD is at $z \approx 5-6$, but this could change if one modifies the models for star formation and feedback.

Using a large set of CHS, Schaye *et al.* [86] examined the impact of various physical models on cosmic SFRD. We show one example of their comparisons in Fig. 6.3, where they turned on/off the SN feedback and metal-line cooling. Without any SN feedback, it is obvious that the simulation overpredicts the observational data points significantly. With SN feedback, star formation is suppressed by a factor of a few to several and becomes more consistent with the observed range of SFRD. Metal cooling enhances the SFRD by a factor of about two at late times. In their

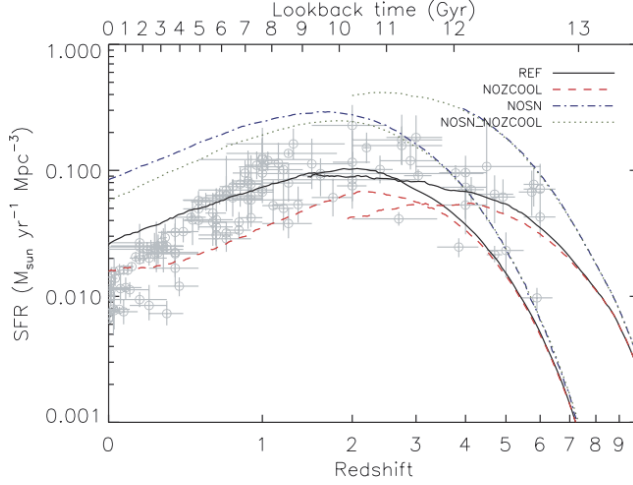


Fig. 6.3. Cosmic SFRD from [86], showing the impact of metal-line cooling and SN feedback. Two sets of four simulations with comoving 25 and $100 h^{-1}$ Mpc boxes are shown: reference run with SN feedback and metal cooling (REF), with feedback but no metal cooling (NOZCOOL), no feedback but with metal cooling (NOSN), no feedback and no metal cooling (NOSN_NOZCOOL). The run with $25 h^{-1}$ Mpc starts star formation at higher redshift due to higher resolution. The SN feedback suppresses SFRD by a factor of few to several, and metal cooling enhances star formation by a factor of a few at late times.

reference model, the peak of SFRD is at $z = 2-3$, which appears to be more consistent with the data points shown in Fig. 6.3. However, observational estimates based on GRB rate and submillimeter (submm) galaxies tend to suggest higher SFRD at $z > 3$ than those estimated from the UV luminosity function of galaxies [87, 88], and there remains a possibility that SFRD may be almost flat during $z \sim 2-6$ [43, 48, 77, 89].

6.8. Galaxy stellar mass function and luminosity function

In CHS, a collection of star and/or gas is identified as a galaxy, and we need to perform “grouping” of these particles to identify galaxies in simulations using a grouping algorithm. The simplest and most common algorithm is the “friends-of-friends” (FOF) [90], which was originally developed to identify DM halos by simply linking all particles that are closer than a certain fraction of initial mean interparticle separation. However, the FOF method is known to overconnect different groups via thin bridges of particles, which is called the “overmerging problem”. Improved versions of grouping algorithms have been developed by many researchers, utilizing a saddle-point overdensity criteria [91], a gravitational binding criteria [92], or phase space information. See Ref. 93 for a comparison of various grouping algorithms.

Once the simulated galaxies are identified using a grouping algorithm, one can compute the luminosity of each star particle using a stellar population synthesis model (e.g., [94–96]) and sum it up to obtain the total spectral output of simulated

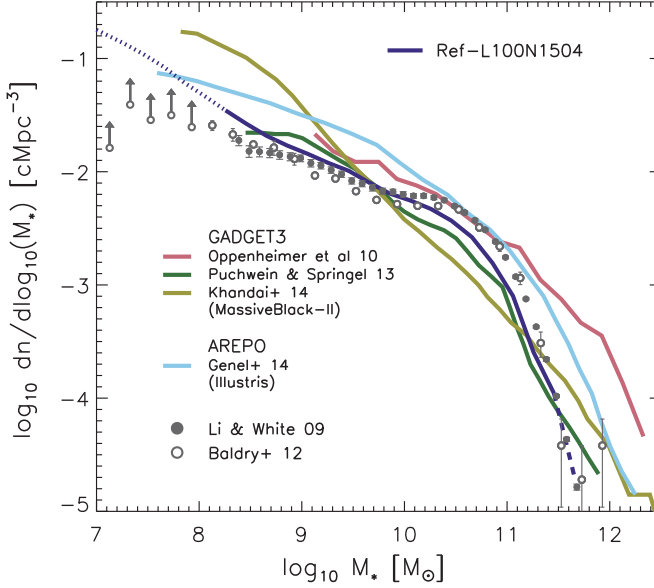


Fig. 6.4. Comparison of GSMF at $z = 0$ between CHS and observational data. Figure taken from [97].

galaxies as a function of cosmic time. This allows us to compute the galaxy luminosity function and check the validity of CHS against abundant observational data from various galaxy surveys.

In Fig. 6.4, we show some examples of simulated galaxy stellar mass function (GSMF) at $z = 0$ compared against observations from Ref. [97]. The shape of the observed GSMF can be described well by a Schechter function, which has a “knee” at $\log(M_*/M_\odot) \simeq 10.8$, an exponential cutoff at the higher mass end, and a flat faint-end slope of $\alpha \simeq -1.2$. We see that different simulations have some variations and do not agree with the observational data completely. Some simulations reproduce the flat faint-end (low-mass end) slope relatively well but misses the exponential cut-off at the massive end, while others agree with the observation at the “knee” but overproduces both low-mass and massive galaxies with a double-power-law-like shape. The shape of GSMF is considered to be controlled by both SN and AGN feedback effects, and it depends on the details of feedback treatment in each simulation as described in Section 6.6.

At higher redshift, the situation appears somewhat different, as the simulations can achieve higher spatial resolution in physical coordinates, and the observational uncertainties increases towards higher redshifts. The faint-end slope α becomes steeper towards higher redshift, from $\alpha \sim -1.2$ ($z = 0$) to $\alpha \sim -1.6$ ($z \sim 3$), and to $\alpha \sim -2.0$ ($z \gtrsim 6$). Figure 6.5 shows a comparison of the rest-frame UV luminosity function at $z = 6-8$ [98], and it has been shown that the simulated luminosity functions and SFR function both agree relatively well with the observational data.

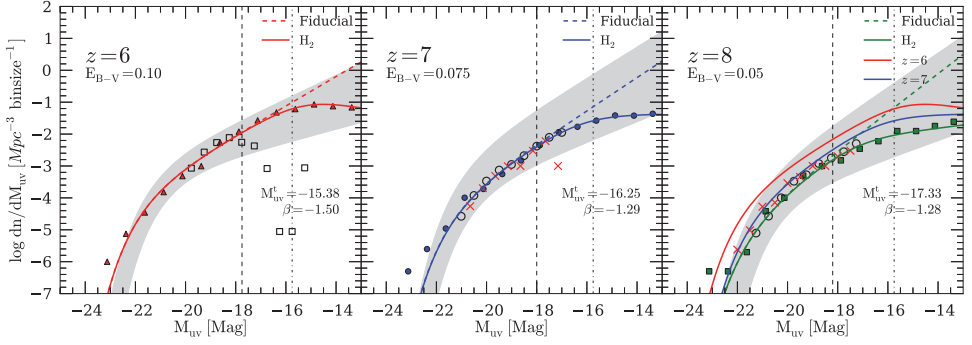


Fig. 6.5. Rest-frame UV luminosity functions of simulated galaxies at $z = 6-8$. The gray-shaded region represents the observed range with its uncertainties, the filled symbols are from simulations, and the solid lines are fits by a modified Schechter function which has an additional turnover at the faint end of $M_{UV} > -16$ mag. The crosses and open circles in the right two panels are also observational data. Figure taken from Ref. 98.

The faint-end slope is quite important for the reionization of the Universe, as it determines the number density of low-mass galaxies that might have high escape fraction of ionizing photons (e.g., [99]) and provide a bulk of ionizing photons necessary for the reionization. An additional flattening of the faint-end slope at rest-frame absolute UV magnitude $M_{UV} > -16$ has also been suggested [98, 100] due to inefficient H_2 formation in these low-metallicity high- z galaxies and/or strong radiative feedback.

By integrating the Schechter function, one can examine the amount of stellar mass contained in each logarithmic bin of galaxy stellar mass and see that star formation was most efficient at the mass scale close to the knee of the GSMF. Behroozi *et al.* [101, 102] showed this by plotting the stellar-to-halo-mass ratio (SHMR) as a function of halo mass, and Fig. 6.6 was obtained by the “abundance matching technique”. Figure 6.6 reveals that the SHMR has a peak at $M_h \sim 10^{12} M_\odot$, and that the star formation was most efficient at this halo-mass scale at $z = 0-5$. At the lower halo-mass end, the SHMR is considered to be suppressed by the SN feedback, and at the higher halo-mass, it is again suppressed by the AGN feedback. While these are the general ideas on the shape of SHMR and GSMF, the mechanism of AGN feedback is not fully understood yet. Usually, it is assumed that the AGN feedback acts as a “negative” feedback owing to a strong injection of energy into the ambient gas from a supermassive black hole (e.g., [103–105]), however, a possibility of “positive” feedback (e.g., jet-induced star formation) has also been pointed out [106–108].

6.9. Galactic morphologies, disk galaxy formation, red sequence, and cold flows

In addition to the statistical properties of galaxies such as GSMF and luminosity function, one of the important goals of computational cosmology is to understand

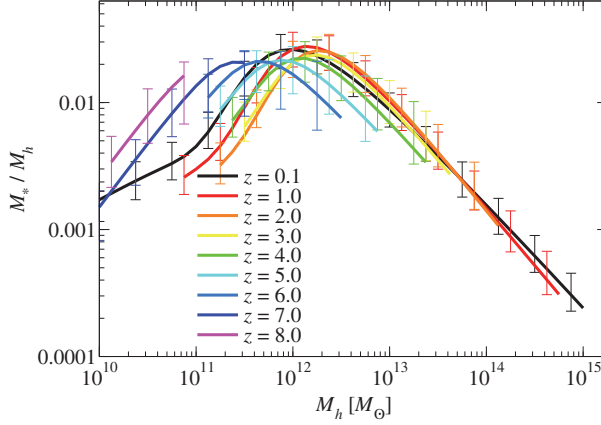


Fig. 6.6. SHMR as a function of halo mass at $z \sim 0-8$ based on an abundance matching technique. One can see that star formation was most efficient in halos with $M_h \sim 10^{12} M_\odot$ at $z \sim 0-5$, and the SHMR is suppressed by the SN and AGN feedback at both lower and higher mass ends, respectively. Figure adapted from [102].

the diverse galactic morphologies, i.e., the emergence of Hubble sequence as a function of time. Traditionally, it was expected that the spherical component of galaxies, such as the bulge and elliptical galaxies, were formed in a monolithic-collapse-like scenario [109] in halos with low angular momentum, while disk galaxies were formed in halos with higher angular momentum [110]. In this simple picture, gaseous halo dissipates and settles into a disk while honoring the angular momentum conservation. Two gas-rich disk galaxies may collide and transform into an elliptical galaxy after a starburst, exhibiting itself as an ultraluminous red galaxy [111–113].

However, more recent works (both observational and theoretical) tell us that the real Universe is more complicated. For example, numerical simulations suggest that a major merger of two disk galaxies may produce both elliptical [103] and disk galaxies [114] with the help of AGN feedback. Observationally, quiescent galaxies contain both bulge- and disk-dominated galaxies [115] and the majority of compact massive galaxies at $z \sim 2$ are disk-dominated [116].

Obtaining proper disk sizes of spiral galaxies was very difficult in the 1990s due to lack of resolution and inadequate treatment of feedback [117, 118]. In the early hydrodynamic simulations, the simulated galactic disks were too small compared to the observations as a result of excessive transfer of angular momentum from gas to DM. Part of the reason might also have been due to numerical issues where commonly used “traditional” SPH was unable to treat the interfaces of multiphase gas well, and excessive angular momenta may have been lost from cold disk to hot halos [119–121]. However, as the improvements were made in all aspects of SPH formulation, numerical resolution and feedback models, the modern simulations in the 21st century began to reproduce large disk sizes that are consistent with observations as shown in Figs. 6.7 and 6.8 [70, 122–126]. In particular, the zoom-in

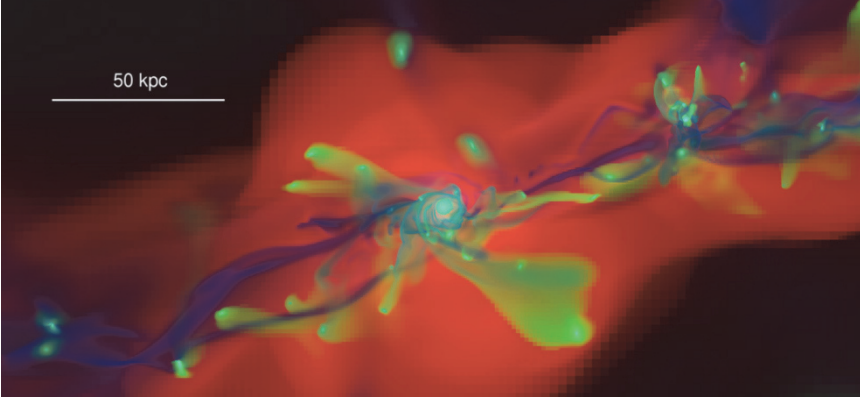


Fig. 6.7. Formation of a disk galaxy at $z \sim 3$. One can see the filamentary “cold flow” (blue) penetrating into the central part of the galaxy, providing pristine gas for star formation. Figure taken from Ref. [125].

technique enabled much higher numerical resolution, better than 100 pc in dense regions where galaxies form, and the treatment of stellar and SN feedback were improved dramatically, resolving the inner structure of galaxies much better than before.

Some CHS using large cosmological box sizes are also beginning to reproduce realistic galactic morphologies and the Hubble sequence at $z = 0$. For example, Refs. 97, 127, 128 have reproduced reasonable population of elliptical and spiral galaxies using the moving mesh code AREPO [129] and GADGET-3 [130] code. One could also attempt to obtain more realistic galaxy images from simulations using a stellar population synthesis code (Fig. 6.8) and performing radiative transfer calculations of stellar light. Schaye *et al.* [97] postprocessed the projected galaxy images with a radiative transfer code SKIRT [131], and obtained the SDSS u, g, r -band images of simulated galaxies accounting for dust extinction. These works still assumed a constant dust-to-metal ratio to account for dust extinction, however, recently more efforts have been made to follow the formation and destruction of dust explicitly in the simulations, leading to more reliable computations of dust extinction [71, 132–135].

The colors of galaxies reflect the age and metallicity of stellar population closely. The massive elliptical galaxies in the present-day universe have ceased their star formation long ago and hence dominated by old, redder stars at $z = 0$, whereas disk galaxies tend to continue star formation smoothly, forming the so-called “blue sequence” on the color–magnitude diagram of galaxies. It is known observationally that the entire galaxy population forms a bimodal color distribution, with “green valley” in the middle [136, 137]. The red sequence (or the so-called “red and dead” galaxies) were difficult to reproduce in CHS [138], but the inclusion of AGN feedback can quench star formation in massive systems and make them sufficiently red [139,

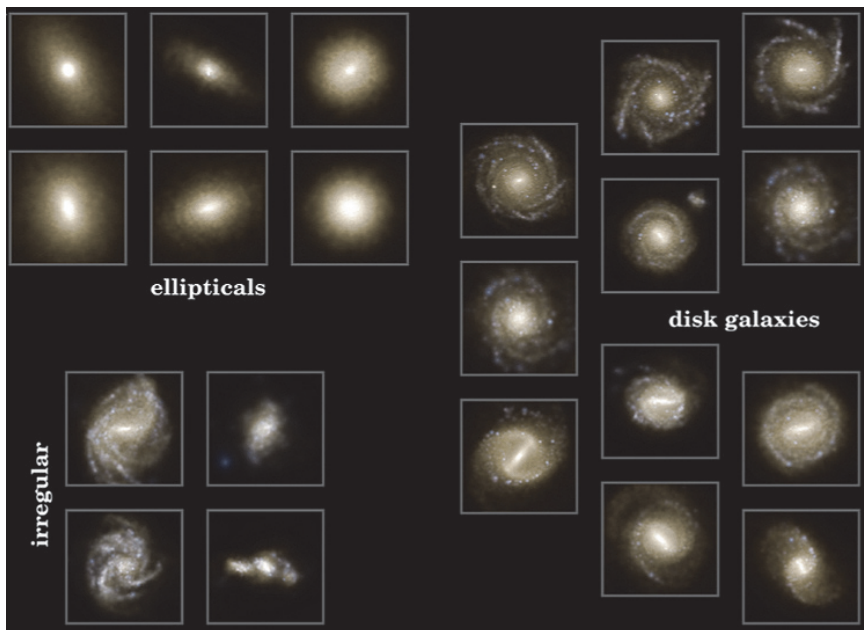


Fig. 6.8. Galaxy images from the Illustris simulations using the AREPO code [127, 129]. A clear Hubble sequence is reproduced at $z = 0$. This simulation was performed in a $(106.5)^3$ Mpc box with more than 12 billion resolution elements. The DM particle mass was $6.26 \times 10^6 M_\odot$, and baryonic mass resolution of $1.26 \times 10^6 M_\odot$. The smallest hydrodynamic resolution was 48 pc, and the gravitational resolution was 710 pc at $z = 0$.

140]. More recent simulations with similar AGN feedback models are becoming better at reproducing the red sequence, but there are still some differences compared to the observed data, such as the tightness and slope of the red sequence, or the balance between red, green, and blue sequence [127, 141]. Reproducing the stellar mass–metallicity relation and $[\alpha/\text{Fe}]$ simultaneously for passive galaxies still seems to be a problem for current CHS [142]. These problems largely stem from our ignorance on how AGN feedback and chemical enrichment work on both large and small scales (see also Sections 3.6 and 3.7 in Chapter 3).

A closely related subject to disk galaxy formation is how galaxies acquire gas when they form. The standard picture until early 1990s was that the infalling gas gets shock-heated by the virial shock when they enter the halo and becomes virialized. However, Refs. 143–145 discovered that some gases do not go through this standard path, but instead penetrate into the galaxy without being shock-heated to $T \gtrsim 10^5$ K. This flow of gas is often called “cold streams” or “cold flow” (see Fig. 6.7) and is considered to be an important channel to provide the gas for galaxy formation and star formation. This is an area of ongoing active research, and the angular momentum transport and entropy variations are being analyzed in various types of

codes using high-resolution zoom-in simulations [146, 147]. Further discussions on this topic can be found in Section 7.6.2 of Chapter 7 and Section 8.6.2 of Chapter 8.

6.10. Summary

As seen in the previous chapters, we have made significant progress in numerical cosmology since 1980s as the speed and efficiency of supercomputers improved. At the same time, we have realized that we need to invest significantly in the development of complex numerical codes to deal with the complexity of supercomputer architecture and various physical processes, such as feedback and detailed atomic and molecular chemistries that are relevant for cooling and star formation. It is truly amazing that we can now reproduce various statistical properties and realistic morphologies of galaxies using CHS (see also Refs. 148, 149 for recent reviews).

In the next decade, cosmological hydrodynamic codes for galaxy formation will deal with more complex physics of feedback from stars, SNe and massive black holes, and our understanding of galaxy formation will be refined further. Current simulations still require some tuning of model parameters for star formation and feedback, but these will be gradually replaced by more self-consistent physical processes as the numerical resolution improves. Inflow and outflow of gas, i.e., the interaction between galaxies, CGM and IGM will be simulated more realistically. A better treatment of radiation transfer (including radiation pressure and force) is also strongly desired for more accurate treatment of feedback processes (see also Chapter 7, Section 7.5.2).

In some sense, we are gradually entering a new era of “*Precision Structure Formation*”, similar to the arrival of “*Precision Cosmology*” era owing to high-resolution measurements of CMB anisotropy. Next generation of galaxy surveys by new instruments (e.g., the Hyper-Supreme-Cam [HSC] and Prime-Focus-Spectrograph [PFS] on Subaru Telescope, JWST, SPICA, TMT, GMT, etc.) will open up new windows to observe the large-scale structure and primordial galaxies at high redshift, and broaden our views deeper and wider. For example, the IGM tomography [150] will give us information on the detailed distribution of gas and metals together with galaxies in the high-redshift Universe. By comparing the results of our future CHS with these new observational data, we will refine our galaxy formation theory, constrain the efficiencies of star formation and feedback by SNe and AGN as a function of redshift and environment, and how galaxies co-evolved with supermassive black holes.

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Chapter 7

Secular Evolution of Disk Galaxies

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In this chapter, we discuss evolution of disk galaxies, focusing on numerical simulations over dynamical and cosmological timescales. Being open systems, galaxies grow and redistribute their angular momentum and mass in response to various factors, internal and external ones, leading to the present state of the Hubble Fork. Galaxies can be studied as mechanical and statistical systems — due to long-range gravitational forces, they are strongly nonlinear systems with a healthy degree of chaotic motions, and capable of forgetting conditions at their origin. Despite their low cosmological average, baryons appear to decouple from the background dark matter on galactic and subgalactic scales, forming a rich variety of objects that can provide feedback to modify their own evolution. This complex interplay between various physical processes is currently at the forefront of astrophysical research using diverse observational methods in tandem with high-resolution numerical simulations.

7.1. Historical introduction

In the history of astronomy which extends well over four millennia, galaxies are relatively new objects. However, the term *galaxy* (galaxies, “milky one” in Greek) precedes its actual “discovery” at least by 2300 years, and was used already in the fifth century BCE to describe the Milky Way appearance in the sky. While in the ancient world, it was suggested by Democritus and repeated by Aristotle, that Milky Way consists of innumerable stars, it was Galileo in 1610 who determined this with the invention of a telescope. Even then, it remained unclear whether the Milky Way is just a distribution of stars or represents a physical system. Immanuel Kant [101] was first to define the Milky Way in modern terms: a collection of a large number of stars held together by their mutual gravity, and having the shape of a (rotating)

disk. Kant also speculated about plurality of “island universes”. William Herschel (and his sister Caroline) actually mapped out the Milky Way [88], being unaware of the effects of gas and dust on its size. This error persisted till the end of nineteenth century (e.g., [102]).

The eighteenth and nineteenth centuries have produced first catalogs of the so-called spiral nebulae [137], and their drawings [87]. Earl of Rosse [160] has argued that they lie beyond our galaxy. Shapley [170] has determined distances to 93 globular clusters using the RR Lyrae stars, and inferred essential details of our galaxy, such that the Sun is at about 25 kpc from its center (today’s value is 8.5 kpc), and that Milky Way must be massive. It was the destiny of the Great Debate of April 26, 1920, to determine (wrongly!) the nature of these objects. The debate was won by Harlow Shapley, who claimed that these objects are “nearby” and lie within the Milky Way, as opposed to Heber Curtis, who argued in favor of them being independent galaxies. As it sometimes happens, the history put everything in the right perspective.

Edwin Hubble, a disillusioned young lawyer who became astronomer, found Cepheids in Andromeda “nebula” in a 1923–24 study, demonstrating that the Milky Way is not alone in the universe, but just one of the many galaxies [94]. Furthermore, Hubble [95] determined distances to 24 nearby galaxies, and their relative velocities — the so-called Hubble Law. It was first obtained theoretically by Lemaitre [116], who also introduced the “Hubble” constant of expansion. This opened the field of observational cosmology. Finally, Hubble introduced the first morphological classification of galaxies, known as the Hubble Fork, in a series of papers (see, e.g., [93], also summarized in [97]).

For completeness, Fritz Zwicky [204] has measured dispersion velocities of galaxies in clusters and concluded that large fraction of their mass is missing in optical observations. Fifty years later, the necessity for this missing mass was verified also by N -body simulations, and Simon White in 1983–84 (see, e.g., [203]) put the last nail into the coffin of alternatives — the missing mass has been finally recognized as the dark matter (DM) dominating the mass in the universe.

7.2. Dissecting a galaxy: Structural parts

The “modern” definition of a galaxy refers to a gravitationally bound object, which includes stars and their remnants, as well as interstellar matter (gas and dust) — all embedded in a DM halo. In the contemporary universe, a galaxy zoo contains two main morphological species: elliptical and disk galaxies. Galaxies which cannot be classified as these are called irregulars. There are obvious differences in appearance between these two classes and within them, and the crucial question is what significance do these differences bear at large. Are they cosmetic or fundamental to our understanding of galaxies? To answer these and other questions, observations,

theory and numerical simulations must be combined. In the following, we shall discuss contributions from all three components, with an emphasis on the latter one.

First attempt to classify galaxies based on their morphology was performed by Hubble, which resulted in the construction of the Hubble Fork diagram, or Hubble sequence. The “fork” originates from a decision to divide the disk galaxies into two subgroups: barred and unbarred (or normal). Superficially, the only difference between these two types is related to the existence of a stellar bar-like feature in the former. The spiral arms extend from the bar-end, instead from the near center in the unbarred branch of galaxies.

Hubble recognized that most galaxies can be assembled from two structural parts, disks and spheroids, and speculated that spheroids predate disks, which have been acquired as a result of evolution — hence early types vs. late types. While the latter statement is not supported by our present understanding, the idea that Hubble sequence is just an admixture of disks and spheroids in varying proportions seems to be correct. Hubble sequence also emphasizes the apparent importance of the spiral arms vs. central spheroidal bulge in disk galaxies.

The early-type galaxies in the Hubble sequence are ellipticals, whose isophote shapes range from being purely circular (E0) to elongated, cigar-shaped (E7). The integer is the rounded up/down $10(1-b/a)$, with a and b being the semimajor/minor axes. The normal late-type galaxies are spiral disks, from Sa to Sd, and SBa to SBd for the barred disks. The $a \rightarrow c$ subsequence reflects increasingly dominant disk component, and decreasing stellar bulge component with respect to the disk. This is measured by the relative light from the disk and the bulge. In addition, along this path, the spiral structure becomes less tightly wound. The d subclass of disks refers to smaller size disks. The intermediate (lenticular) S0 and SB0 disks lack spiral structure, still being barred and unbarred. Galaxies which cannot fit within this scheme are called irregulars (Irr). Lastly, one distinguishes between grand-design spiral structure — typically, a well-developed pair of arms, and flocculent spirals, exhibiting numerous irregular spiral fragments.

This original division into Hubble types relies on the galaxies in the contemporary universe. How does it depend on the environment where the galaxies reside? First noticed by Hubble and Humason [96], the dominance of the early morphological types, i.e., ellipticals, in the dense environment of galaxy clusters has been confirmed by future observations. This density–morphology relation is well established now (see, e.g., [51]), but does it evolve with redshift?

In the local universe, the spiral disk galaxies constitute a majority, followed by lenticular galaxies, and by ellipticals. About 10% of galaxies are classified as peculiar. But already at $z \sim 0.6$, the fraction of spiral disks declines by more than a factor 2, while the fraction of peculiars increases five-fold, and the abundance of lenticulars and ellipticals changes much less (see, e.g., [47]). This trend is observed also at higher redshifts [25]. Explaining the formation of the Hubble sequence, both

qualitatively and quantitatively, is the focal and challenging point of contemporary research in galaxy evolution.

So, the dominant galactic morphology does change with redshift, but does it depend on other parameters, such as baryonic mass of galaxies, properties of parent dark matter halos, gas fraction, environment, presence of central supermassive black hole (SMBH), and more? As one expects these parameters to change with redshift, galaxies are expected to evolve. This evolution can be crudely separated based on its characteristic timescale. If changes occur on the crossing time or orbital time, they constitute *dynamical* evolution. On the other hand, if they occur on a much longer timescale, the evolution is called *secular*. Here, we shall focus on the secular evolution of galaxies, yet in such complex systems like galaxies, complete separation between timescales is impossible.

Observationally, measurements of galactic masses require a substantial effort, even if one asks only for stellar masses. The latter masses are typically replaced by absolute luminosities, which require the knowledge of distances, and mass distribution function for galaxies is frequently substituted by galaxy luminosity function. However, a substantial progress has been made in recent years in determining the galaxy mass function as well, especially for its massive end (see, e.g., [28, 52, 72]).

Galactic morphology shows a tight correlation with galactic mass. Various structure parameters, such as concentration index, half-light surface brightness, surface mass density, etc., show correlation with the absolute magnitude and stellar mass in galaxies (see, e.g., [103]).

Additional factors are known to affect the galactic morphology, such as feedback from stellar evolution and from active galactic nuclei (AGN), redistribution of mass and angular momentum, etc. Finally, various processes can drive a galaxy to the configuration when no steady state is possible, and the morphology changes abruptly.

In order to understand galaxy evolution, one can attempt to emphasize various factors which play a dominant role in this evolution. These factors can be mechanical and statistical. In the following chapters, we attempt to provide systematics in these processes.

7.3. Disk galaxies as mechanical systems

Morphological differences between elliptical and disk galaxies are based on substantially different kinematics. The former are supported largely by random motions, while the latter by rotation. Low dispersion velocities in the disks, compared to tangential velocities, mean that the disks are “cold” and explain why they are geometrically-thin, with $c/a \sim 0.1$, where a and c are semimajor and semiminor axes. As such, one expects disks to support circular or elliptical stellar orbits, with a small amplitude vertical oscillations. This is, however, an overly simplification, as we shall see below.

Galactic disks are embedded in DM halos, which appear to have triaxial¹ shapes at the time of formation (see, e.g., [2, 10, 15, 16, 53, 171]), and are supported by random motions, rotation being negligible. Indirect observational evidence of DM halo shapes comes from gas kinematics in disk galaxies, their polar rings, warps, and gravitational lensing, but the results are rather inconclusive.

Some clues nevertheless exist. Residual potential axial ratios (both flatness and prolateness defined in the footnote) of about 0.9 in the DM halos are plausible, even in present-day galaxies (see, e.g., [112, 150] for the Milky Way). The position angle twist of the X-ray isophotes detected by Chandra in NGC 720 has provided an independent evidence for the DM halo triaxiality. This, however, has not been confirmed by the stellar isophotes [29]. Moreover, a kinematic study of a planetary nebula system pointed to a degree of prolateness, with $T \sim 0.985$, $b/a \sim 0.791$, and $c/a \sim 0.787$ for the DM halo of elliptical galaxy NGC 5128 [145]. Hence, the statistical significance of *contemporary* DM halo triaxiality is not clear, although some individual halo shapes are compatible with being mildly prolate even at $z = 0$. Whether disk galaxies differ in this respect from elliptical galaxies is not clear as well. We conclude that the prolateness of contemporary halos appears to be insignificant.

Definition of a mechanical system follows from celestial mechanics, and uses perturbed orbits and no chaos. It will be helpful at this point to introduce definitions of regular and chaotic systems (see also Chapter 7.4). A regular dynamical system is one whose evolution depends uniquely on its initial conditions. On the other hand, a chaotic system is one which is highly sensitive to the initial conditions. This effect is conventionally known as the Butterfly Effect [24, 121].

7.3.1. *Collisionless dynamics: Stars and dark matter*

The most straightforward way to follow motions of stars and DM particles is defining their orbits. Orbits have been introduced first in order to quantify motions in the Solar System, both within geocentric and heliocentric cosmologies (Pythagoras, Aristarchus). These idealized orbits required corrections to remove discrepancies with observations — this led to the epicyclic theory of planetary motion, proposed by Apollonius of Pergas in the third century BCE, and further developed and used by Hypparchus of Rhodes and Ptolemy of Thebaid (second century CE). The epicyclic motions have been fully implemented in the Antikythera machine — first portable analog computer built on the planet (circa end third century BCE) and found in the shipwreck in 1901. The contemporary orbit theory starts with Isaac Newton [141] and its development was nicely delineated by Donald Lynden-Bell [127].

¹Following [15], the triaxiality is defined here as $T = [1 - (b/a)^2]/[1 - (c/a)^2]$, where c/a is the halo's polar-to-longest equatorial axis ratio and b/a is the equatorial axis ratio; $T = 1$ corresponds to a prolate halo, while $T = 0$ to an oblate one. The halo *flatness* is defined as $f = 1 - c/a$ and its *prolateness* (i.e., equatorial ellipticity) as $\epsilon_h = 1 - b/a$.

Dynamical evolution can sometimes be observed directly, especially when galaxies interact and merge. Its characteristic timescale is of the order of a crossing time of the system, i.e., $\tau_{\text{dyn}} \sim R/v_{\text{ff}}$. Here, R is the characteristic size of the system and v_{ff} is the free-fall velocity of a test particle in its potential. Secular evolution of galaxies can be only studied observationally indirectly, by producing statistical samples of galaxies. Here, numerical simulations are indispensable. Introduced by Holmberg (1941, [91]) via an analog computer based on measurement of radiation flux from ordinary light bulbs, numerical simulations serve as experimental component in astronomy, supplementing observations and theory, and responsible for fast progress in various fields.

While direct stellar collisions occur only under extreme conditions (see, e.g., [73]), stellar encounters which cause small deflections in stellar orbits cause energy and angular momentum transfer due to gravity being a long-range force. The resulting two-body relaxation timescale for spheroidal N -body self-gravitating systems with dispersion velocities σ and point (stellar or DM) particles with masses m is $\tau_{\text{rel}} \sim (N/8 \ln N) \tau_{\text{dyn}}$.

Hence, for small N , the two-body relaxation is comparable to dynamical time. Elliptical galaxies (and DM halos) have τ_{rel} larger than Hubble time and must be modeled with a sufficiently large N to avoid numerical artifacts associated with a short two-body relaxation. In rotationally supported systems, i.e., galactic disks, τ_{rel} will be substantially shortened because particle encounter velocities are much smaller than in spheroidal systems (still very long!), and, therefore, will be deflected much more efficiently (see, e.g., [161]). But the associated relaxation in strongly flattened rotating objects does not have the same global meaning as in objects supported by random motions, and rather operates on spatial scales corresponding to the disk thickness. Hence, stars and DM in galaxies and their halos behave as collisionless fluids.

The prevailing symmetry of gravitational potential is crucial in understanding the internal kinematics and dynamics of stellar systems and, therefore, their evolution. In disk systems, which are supported by rotation, the degree of axial symmetry determines the prevailing families of orbits (Section 7.4.1). The two major and most common factors are spiral arms and bars. The former are density waves propagating in a differentially rotating disks. The individual stars cross the arms, being slowed down only slightly by a weak perturbation in the gravitational potential — no stellar orbit trapping occurs. On the other hand, stellar bars are self-gravitating entities and trap majority of stellar orbits within the disk region where they reside, thus fundamentally changing the shapes of otherwise disk orbits. This is possible because of a substantial change in the angular momentum of these orbits.

7.4. Disk galaxies as statistical systems

Neglecting the gas component in galaxies, they can be considered as N -body systems, consisting of stars and dark matter. For most galaxies, the number of stars,

$\sim 10^8\text{--}11$, is large, and the number of DM particles in the parent halos is even larger. Clearly, the N -body problem cannot be solved analytically, and numerical approach has proven to be indispensable. It is also possible to study the galaxy properties using the statistical approach. Observations provide us with information about the present dynamical state of disk and elliptical galaxies. To deduce the past and future evolution using this information is very difficult, and rather next to impossible. Hence, based on observations, we cannot directly determine the fraction of chaotic orbits in a system — numerical simulations play the crucial role here.

7.4.1. *Order and chaos*

Galactic gravitational potentials give rise to both regular and irregular (chaotic) orbits. While definition of an orbit did not change since antiquity, the systematic study of orbits in various potentials brought up the issue of self-consistency — the stacking of individual orbits should provide the density response which is in tandem with the underlying gravitational potential. This is a reflection of requirement to satisfy the Poisson equation in self-gravitating system, but goes a step ahead by demanding that density distribution will be related to the dynamical state of the system. It appears that one gains a substantial knowledge about the morphology and dynamics of a system (i.e., galaxy) by analyzing the families of orbits which comprise the system.

Orbits can be divided into periodic and quasi-periodic ones, which represent regular orbits, and into chaotic orbits. They can be studied in fixed and varying potentials. Regular orbits in three-dimensional (3D) space are those that can be separated into three independent periodic motions. The great importance of these orbits lies in that they are usually stable, and form the backbone of a density distribution and, therefore, of the underlying potential. Stable orbits trap the so-called quasi-periodic orbits in their neighborhood — the latter possess additional secondary frequencies in their oscillations around the periodic orbits — altogether they define the basic structure of the galaxy. An example of a periodic orbit is a circular orbit in the equatorial plane of an axisymmetric potential. On the other hand, irregular or stochastic orbits are not made out of periodic motions and their domain is limited only by energy conservation. In the phase space, the regions populated by chaotic orbits can be separated, or connected, insignificant or dominating — contributing to the loss of structure and dissolution of the system.

Orbits which are formed by low-amplitude perturbations of stable circular orbits can be treated formally by the epicyclic approximation (see, e.g., [19, 40]). They are characterized by two frequencies, the angular frequency Ω , corresponding to the motion of the “guiding” center, and the radial epicyclic frequency κ , measuring the radial departure from the guiding center. In 3D, a third frequency ν is related to the vertical oscillation of the orbit. When Ω and κ , and Ω and ν are commensurable, i.e., their ratios are rational, the orbit is closed. Otherwise, it forms a rosette. All closed orbits are resonant and periodic in the inertial frame, e.g., $\kappa/\Omega = n/m$, where

n (number of radial oscillations) and m (number of revolutions) are integers. In the noninertial frame which tumbles with pattern speed Ω_p , the resonance is between $\Omega - \Omega_p$ and κ , i.e.,

$$\frac{\kappa}{\Omega - \Omega_p} = \frac{n}{m}, \quad (7.1)$$

and the orbit closes in the rotating frame. The most important resonances are the low-level resonances, $n/m = \pm 2/1$. These are the Lindblad resonances, with $+$ corresponding to inner Lindblad resonances (ILR), and $-$ to outer Lindblad resonance (OLR). Corotation is another important resonance, with $\Omega = \Omega_p$.

In Eq. (7.1), $\Omega - \kappa/2$ is the precession frequency of a stellar orbit. When it is equal to Ω_p , we obtain an orbit which is in resonance with the perturbation frequency. Figure 7.1 provides examples of main resonances for various rotation curves in the disk. The ILRs occur within the corotation radius, while OLR lies outside. Only one OLR exists while none-to-few ILRs can occur.

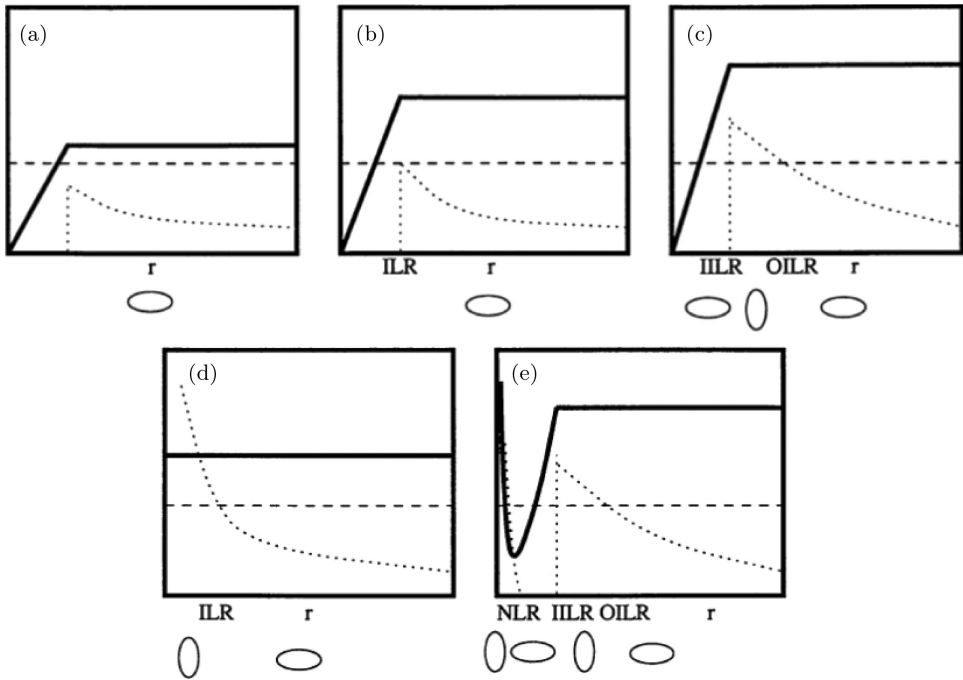


Fig. 7.1. Schematic appearance of linear resonances in a galactic disk for various rotation curves $v_\phi(r)$ (solid lines) within the corotation radius. The disk is perturbed by a bar or spiral arms. Dashed lines give the pattern speed Ω_p of the perturbation; dotted lines represent the orbital precession frequency $\Omega - \kappa/2$ (see text). Ovals provide the orbital response to the perturbation major axis — i.e., horizontal ovals support the perturbation and vertical ovals weaken it. Resonances are abbreviated by inner ILR (IILR), outer ILR (OILR), and NLR (nuclear Lindblad resonance). (From [178].)

All frequencies are generally functions of a position, and κ can be expressed in terms of Ω and its radial derivative. Because $\Omega - \kappa/2$ has a special significance, we mention a number of possibilities here. If the galaxy is very centrally concentrated or hosts an SMBH, $\Omega - \kappa/2$ increases indefinitely with $r \rightarrow 0$, and at least one ILR is present, e.g., nuclear Lindblad resonance (NLR). Alternatively, if the galaxy has a density core in baryons and DM, $\Omega - \kappa/2$ tends to zero at the origin, and ILR can be absent, although this depends on additional factors, such as the degree of nonaxisymmetry in the mass distribution and Ω_p . A caution must be exercised because the above formalism is limited by small departures from the axisymmetry in the background potential, e.g., spiral arms and very weak bars — perturbations are linear or quasi-linear when asymmetry is less than 10% of the radial force. Typical bars are nonlinear perturbations of 100%. Under these conditions, $\Omega - \kappa/2$ is lowered and the ILR(s) are absent. Despite this, linear analysis can show their presence erroneously. Effects of a varying bar strength on the shapes of orbits are shown in Ref. 39.

7.4.1.1. *Families of orbits*

The simplest families of orbits in barred disk galaxies are low-order planar periodic orbits inside the CR. The search for such orbits is restricted to initial conditions in the xy -plane $x = z = \dot{y} = \dot{z} = 0$, and the orbits start on the y -axis, perpendicular to the bar major axis. An example of a characteristic diagram for such orbits in the bar frame is shown in Fig. 7.2 [81], where y represents the crossing (and starting) point of an orbit, and E_J is the Jacobi energy of an orbit. This energy is conserved in the rotating nonaxisymmetric potential, e.g., in the frame of the bar, $E_J = E - \vec{\Omega} \cdot \vec{L}$. Here, E is the energy in the inertial frame, $\vec{L}$ the angular momentum, and $\vec{\Omega}_b$ is the bar pattern speed. The zero velocity curve (ZVC) delineates the region accessible to the orbit. It becomes vertical at the CR, then opens up outside the CR. Each point on the characteristic diagram, therefore, corresponds to a single period orbit.

The orbits are arranged in families represented by various characteristic curves on the diagram. Stable orbits are shown as solid lines, while unstable orbits (or unstable sections of these curves) are given by dotted lines. The notation for these orbital families used here is that of Ref. [39]. Namely, the x_1 family consists of orbits elongated along the bar, and rotating around the center in the same sense as the bar, i.e., direct orbits. In the bar frame, they move radially out twice for one rotation, 2/1. The population of these orbits is the main family which defines the bar, and to a large degree its shape and structure. The x -extent (along the bar) of the x_1 orbits increases monotonically with E_J from the center, out to the point of bifurcation, where 3/1 family of orbits starts. The y -extent of x_1 family is not monotonic, and has a local maximum around $E_J \approx -5.7$. The eccentricity of orbits in this family also increases monotonically in Fig. 7.2 [81], but other possibilities exist as well, depending on the bar strength.

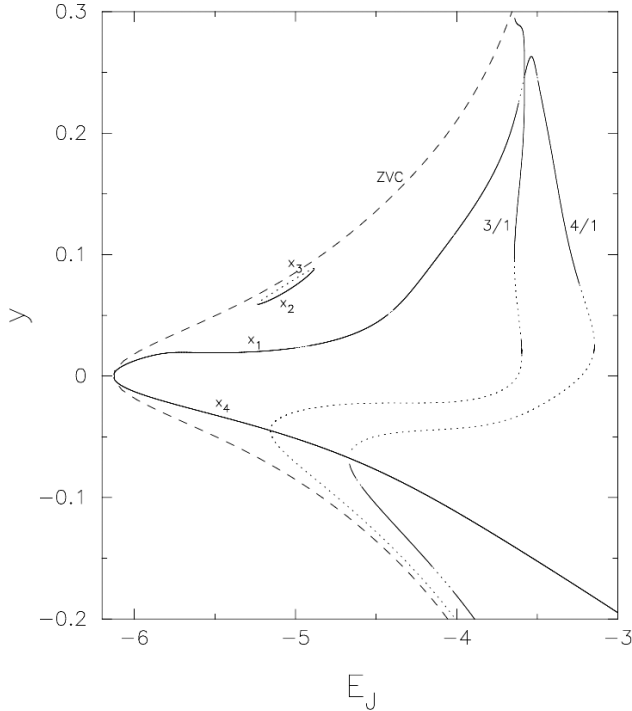


Fig. 7.2. Characteristic diagram for planar periodic orbits inside the corotation radius of a barred stellar disk. The main families have been labeled using notation in Ref. 39 — direct (x_1) and retrograde (x_4) along the stellar bar; x_2 and x_3 direct orbits elongated perpendicular to the bar. The ZVC is given by dashed lines, and stable/unstable sections are represented by solid/dotted lines. (From [81].)

Further, the x_1 orbits family turns downward and changes into 4/1 family. The 4/1 family curve changes from direct to retrograde, and then to 3-periodic family, before meeting the retrograde family x_4 (see, e.g., [3, 81, 167]).

Next, the x_2 family of orbits are direct orbits as well, but elongated perpendicular to the bar. They are present only if the system harbors an ILR. The range in E_J of this family depends on how many ILRs exist — for a single ILR, the family extends all the way to the center, but if two ILRs exist, it is found between the resonances only, e.g., as in Fig. 7.2. In fact, the extremes of the x_2 family on the E_J axis define the positions of the ILRs. The x_2 orbits are less elliptical than x_1 , which is important when one discussed their ability to trap and retain gas. The adjacent family of orbits squeezed between the x_2 and the ZVC are the x_3 orbits, direct and unstable, and, therefore, we avoid discussing them here, although such orbits can become important when one involves the 3D orbits. These rules explain the behavior of orbits also, as shown in Fig. 7.1.

Finally, the x_4 family of orbits is 2/1 and retrograde with respect to the bar tumbling, and slightly elongated perpendicular to the bar. Hence, when bars are

present, such orbits should be populated only sparsely. Otherwise, this family can be important in bar dissolution.

The vertical shapes of periodic orbits are important when one follows the bar shape evolution in the xz -plane, and determine the various aspects of vertical buckling instability in the bars, e.g., Section 7.5.1.2.

7.4.1.2. *Chaotic orbits*

Breaking of axial symmetry in a galaxy, e.g., by a bar or triaxial DM halo, introduces gravitational torques which trigger accelerated redistribution of mass and angular momentum. These torques become even more important when both bar and triaxial halo are present, causing interaction of two gravitational quadrupoles. The shapes of stellar bars and DM halos must be supported by their orbital structure. If the system is a long-lived one, it must also be in a steady state. This requirement brings up the issue of integrals of motion. Integral of motion is typically associated with spatial symmetries in a dynamical system [57, 136]. These symmetries are not limited to simple spatial ones, and lead to global integrals of motion which can maintain the triaxial structure, e.g., most of the Stäckel potentials [49]. For example, in a system which is not centrally concentrated, the potential can be approximated as a quadratic form, and the motion is separable and even linear in Cartesian coordinates [58]. On the other hand, centrally concentrated systems do not have such symmetries, and no global integral of motion exists there. Introduction of a stellar bar (or similar nonaxisymmetric perturbations) in such systems will lead to formation of chaotic orbits there.

Chaos is an instability whose timescale can vary from about a dynamical one to a substantially longer timescale — its presence restricts the Laplace determinism to a limited time, and even this is an approximation. An example of a very long timescale for development of chaos is the Solar System.

A possible way to quantify the chaotic behavior is by means of the Liapunov exponents [30, 117, 118]. Bounded orbits in a gravitational potential can be characterized by such exponents — their number is equal to the number of phase-space coordinates. These exponents measure the rate of divergence of two neighboring initial points of a dynamical system. While this method is well known in nonlinear dynamics, only few attempts have been made to apply it to realistic galactic potentials [195].

The first self-contained description to obtain the Liapunov exponents in this context was given by El-Zant and Shlosman [57, 59]. Specifically, and in simplified terms, the asymptotic rate at which the distance in the phase space between initially adjacent trajectories increases compared to the exponential is determined by the Liapunov exponents. This distance, starting with initial conditions around $\vec{X}(0)$, can be defined as $||\delta\vec{X}[t, \vec{X}(0)]||$. A Liapunov exponent as well as its inverse — a characteristic exponential timescale — can be defined with respect to each initial condition $\vec{X}(0)$ and perturbation $\delta\vec{X}(0)$. Consequently, this creates

a mapping between the space of initial conditions and the stability associated with them.

The exponents converge to zero, if $\|\delta\vec{X}(t)\| \sim t$, as in the case of a regular motion. Alternatively, if $\|\delta\vec{X}(t)\| \sim \exp(t)$, as in the case of an unstable system, the maximal exponent tends to a finite limit. An aperiodic orbit with at least one positive Liapunov exponent is chaotic, i.e., stochastic.

The actual situation can be much more complex, and a system initially confined to 2D (two dimension) can become fully 3D as a result of, e.g., a local instability. Another issue is that for very limited time intervals, the clean separation between regular and chaotic orbits based on Liapunov exponents is nearly impossible. Finally, in order for the system to be truly chaotic, mixing of orbits must occur on the timescale of a few Liapunov times. Note that a dynamical system wandering in the phase space can be intermittently chaotic and regular.

Analytic methods are not very efficient in determining the chaotic orbits. The numerical orbit integration has resulted in a substantial understanding of orbital dynamics in the mean field approximation of galactic potentials [40]. Various numerical methods have been developed, e.g., Poincare map (surface of sections), which exhibit intersection of orbits with specific lower-dimension subspace (see, Fig. 7.3) [19].

7.5. Internally-driven evolution in disk galaxies

In this section, we focus on the secular evolution of disk galaxies driven by nonaxisymmetric features on various spatial scales, from global to local ones. Such departures from axial symmetry include various shapes of DM halos, galactic bars, spiral arms, etc. Galactic bars, without doubt, appear to be the main *internal* engines of galaxy evolution. They facilitate angular momentum and mass redistribution, and trigger or damp star formation [7, 13, 164, 167, 176]. While studied over more than five decades, many details of bar formation and evolution are still pending. Substantial progress has been also achieved in addressing the dynamical effects of DM halos on disks, despite clear difficulties of DM “observations”. These effects on barred disks can be substantial, as we discuss below.

7.5.1. Angular momentum and mass redistribution

7.5.1.1. Dark matter cusps

High-resolution numerical simulations have shown evidence for a cuspy density profile of DM halos, $\rho(r) \propto r^{-\alpha}$, with $\alpha \sim 1 - 1.5$, down to the resolution limit (see, e.g., [53, 76, 108, 140], hereafter NFW). NFW provided a parametric density profile, claimed to be a universal one, independent of halo mass. It has been characterized by $\alpha = 1$ cusp. Theoretically, it has been shown that such cusps can form from the cold gravitational collapse in an expanding universe [61, 119].

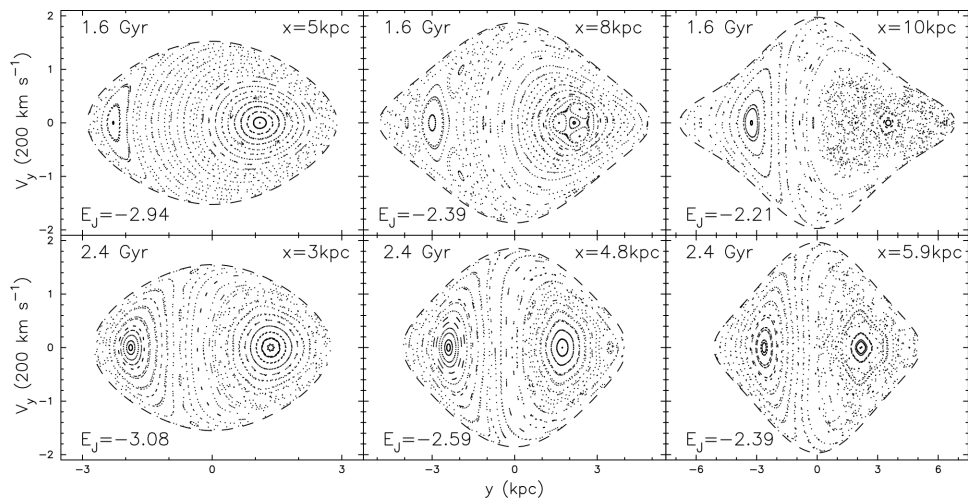


Fig. 7.3. Surface of sections (Poincaré map) diagrams showing a stochastic orbit-dominated strong bar (in the y - v_y plane), which experiences a vertical buckling instability (Section 7.5.1.2), and as a result evolves into a shorter and weaker bar which contains a larger fraction of regular orbits in the midplane, $z = 0$. The fixed points represent the parent orbits which are surrounded by regular orbits forming closed curves around them. The axes x and y are oriented along the major and minor axes of the bar. The retrograde orbits are found on the $y < 0$ side, while the prograde orbits are on $y > 0$. At the fixed Jacobi energy, E_J corresponds to R_b — the bar end (right column), $0.8R_b$ (middle column), and $0.5R_b$ (left column) — made at two different times, $t = 1.6$ Gyr (upper panels) and $t = 2.4$ Gyr (lower panels), when the bar size has dropped from $R_b \sim 10$ kpc to below 6 kpc. Deeper inside the bar, the direct and retrograde orbits dominate the phase space. Here, distances to the center are given in the right upper corners. Two conclusions can be made. Namely, *regular* orbits occupy a much smaller fraction of the phase space in the outer stronger bar (upper right panel) compared to the dissolved outer and overall weakened bar (lower right panel). Moreover, the stochastic region expands inward from the CR of the bar, dissolving its outer part, outside ~ 5.9 kpc. (From [132].)

However, being “thermodynamically” unstable, such cusps can be dissolved by a dynamical friction with clumpy baryons and form a flat DM density core, as shown in numerical simulations [56, 60, 154] and theoretically [62]. A byproduct of this process is the formation of a baryonic cusp replacing the DM cusp, although this depends on the feedback from SF and AGN. Depending on the initial conditions, the total density distribution may become either more or less centrally concentrated.

Alternative options for DM cusp destruction are baryon energy feedback [134] and stellar bar–DM halo interaction [200]. The latter option, however, has been questioned directly [169] and indirectly [54].

7.5.1.2. Stellar bars

Bar instability is probably the most important instability in the life of a rotating dynamical system. It was first studied along the Maclaurin sequence of rotating self-gravitating fluids where the system reaches a bifurcation point beyond which

a spontaneous symmetry breaking occurs. This symmetry breaking corresponds to phase transitions of various orders in self-gravitating fluids and collisionless systems [18, 32, 35]. But it represents essentially a universal way the systems get rid of their angular momentum in various objects, from neutron star formation to galactic disks, to seed SMBHs, and beyond. The “classical” bar instability reflects a spontaneous symmetry breaking in rotating and originally axisymmetric system. It is a global instability because already in the linear stage its wavelength is comparable to the size of the system. Analytic approach to disk stability fails to recognize and misses this instability because it is based on the local approximations [19]. Originally detected in numerical simulations [90], it has been interpreted in terms of a swing and other amplification mechanisms of density waves [193]. In the absence of an analytical treatment, numerical investigation of bar instability is currently the only viable path.

While the bar instability in (collisionless) stellar or (dissipative) gaseous systems is robust, the exact conditions for it to develop are rather murky. Empirically, based on actual or virtual experiments, various parameters have been suggested, e.g., the ratio of the bulk kinetic-to-gravitational potential energies ratio, $K/|W|$ [142], or its modifications [36]. These early simulations already found that the rise time for the bar instability depends on dispersion velocities in the disk and on the disk-to-halo mass ratio [4, 193]. This list, however, is not a complete one — the DM spin is important as well [120, 163].

Despite difficulties with analytical approach, early progress was made in understanding the resonant character of angular momentum redistribution in the disk-halo system [125, 194]. The angular momentum flow was found to be dominated by the low m resonances: the disk ILR is the main emitter, followed by the Ultra-Harmonic Resonance (UHR) and other resonances inside the CR, while it is absorbed mainly by the OLR and other resonances outside the CR. The DM halo absorbs at all resonances.

Disk bar: We start discussing mutual interaction between galactic bars and disks. The latter consist of two components, roughly speaking, stars and gas. These components respond in a different fashion to nonaxisymmetric perturbations. In reality, one should remember that the disk stars have different dispersion velocities, and their response, in principle, depends on how “hot” is the particular stellar population. Likewise, the gas consists of a number of components, from clumpy Giant Molecular Clouds (GMCs), to a rather continuous warm interstellar medium (ISM). Unfortunately, resolution of numerical simulations allows either to follow the ISM in great detail on a few pc scale, or to follow the galaxy evolution on a few kpc scale. In the latter case, a number of crucial physical processes, such as star formation, must be dealt at the subgrid level, which oversimplifies them. Not only numerical but also theoretical issues related to many of these processes make the simulated evolution a model-dependent one. However, numerical simulations do catch many of the essential details of disk evolution.

Bars reflect the ability of a rotating dynamical system to reduce its angular momentum by either redistributing it within the system or transferring it to another (interacting) system. Bars can develop spontaneously or be triggered. The nature appears to use both options, and the observed galactic bars on all spatial scales can have various origins. Among disk galaxies, bars are ubiquitous, yet of a widely ranging strength. If we use the simplest observationally motivated definition of the bar strength, i.e., their face-on or deprojected ellipticity, $\epsilon = 1 - b/a$, where a and b are their semimajor and minor axes, about equal fractions of bars are strong, medium strong, and weak [167]. Here, we separate the bars at $\epsilon \sim 0.4$ and 0.25 . Some disks appear unbarred, but deeper infrared imaging is required to verify this. Keeping in mind that bars can appear and disappear (although not easily!), the fact that majority of disks are barred tells about the bar phenomenon as being a truly universal one.

Detection of stellar bars requires addressing the distribution of the intermediate stellar population in disks and can be done most reliably in the nearby universe in the near-infrared, K band. At higher redshifts, the resolution problem becomes important. First attempts to estimate the bar fraction at $z < 1$ have led to a claim that bars disappear beyond $z \sim 0.5$ (see, e.g., [1]). However, subsequent works did not support this claim. At least for large bars, which can be detected till $z \sim 1$, the bar fraction remains unchanged within a factor of 2 [100, 172]. At higher redshifts, a number of contradictory processes have been proposed, which anticipate both larger and smaller bar fractions. Numerical simulations, on the other hand, while clearly not being able to account for all processes yet, show disk galaxy-dominated universe at $z \sim 10$, at least for massive galaxies of stellar mass $M_* \gtrsim 10^9 M_\odot$, with some prominent bars [159].

Numerical simulations of isolated galaxies almost always start with axisymmetric disks embedded in DM halos, and evolve over few Gyrs. We first discuss simulations following collisionless components, stars and DM only, then turn our attention to the gas presence. Some, usually early simulations used even more simplified approach, assuming fixed DM halo gravitational potentials (see, e.g., [22]) because of limited computational resources, while others (see, e.g., [14, 17, 41, 80, 166, 176]) used “live” halos. The resulting evolution differs substantially in both cases because a fixed halo is unable to absorb any angular momentum from the disk.

The angular momentum flow has been confirmed to drain the angular momentum from the bar region and deposit it in the outer disk, beyond the CR, in tandem with analytical calculations listed above. However, the disk mass fraction is quite small beyond this resonance for large-scale bars, and therefore this transfer quickly saturates — the flow is then directed to the DM halo. The reason why does the outer disk respond first is the result of being “cold” compared to the halo. However, DM halo typically has mass equal to that of the disk within its outer radius and a low angular momentum compared to the Keplerian support. Hence, it is capable of serving as a sink — the disk being the source of J [7, 8, 133, 166, 197]. While this

seems to be natural, it appears that even halo can saturate in this process, as we discuss below.

The dual role of spheroids in angular momentum redistribution has been pointed out by Villa-Vargas *et al.* (2009 [197]). Namely, during the bar instability, more massive halos slowdown the bar formation, while subsequently, during secular evolution of bars, more massive spheroids lead to stronger bars.

Even with collisionless stars only in the disk, one observes a substantial mass redistribution in response to the secular bar action. Gravitational torques act on stars and this action over extended time periods pushes older stars inwards [54, 78]. The surface density of the inner disks exceeds that of an exponential disk, thus contributing to the formation and/or growth of galactic bulges, defined as disk bulges in contrast to classical bulges [9, 111]. The outer disk, however, becomes more extended with increasing radial scale-length, depending on velocity dispersions in the disk [42].

The central mass concentration grows much faster and by a large factor of ~ 2 , even during a short period of bar instability [54]. On the other hand, formation of the outer spiral arms, which is related to the disk–halo angular momentum transfer, leads to the radial “puffing” of the disk, sometimes quite substantially.

Disk–halo interaction can be dramatically amplified by the presence of non-axisymmetric features, such as halo triaxiality or the presence of galactic bars. Additional factors, such as centrally-concentrated density distribution and clumpiness in the mass distribution, can further modify the underlying dynamics. Galactic bars on scales larger than $\sim \text{kpc}$ are dominated by their stellar component. Early theoretical works have already realized the prime importance of bars on the angular momentum redistribution between various disk and spheroidal components [125, 126, 194, 199]. Most importantly, the dominant role of resonances in this process has been clearly shown.

First published simulations displaying flow of angular momentum from a barred disk to DM halo while providing few details due to a low resolution nevertheless capture the essence of the process [41, 166]. Confirmation that resonances facilitate the angular transfer from the disk to DM halo came from the analysis of three representative numerical models of isolated disk galaxies embedded in various mass DM halos [8]. Figure 7.4 exhibits the prevailing contribution by the lower resonances to the angular momentum flow from the disk to the DM halo. The disk loses J , primarily via its ILR, while halo gains it via the CR. The angular momentum transfer away from the resonances is small. This is confirmed in other models [31, 133]. Two methods have been used for this purpose — spectral analysis of the orbits in a fixed potential [8, 133] and in a live potential [31]. The latter approach suffers from limited integration time, $\sim 1 \text{ Gyr}$, which leads to wider resonances and overestimates their trapping ability. Furthermore, the rate of J flow in numerical barred disk–halo systems has been directly extracted from N -body simulations in cylindrical shells [120, 197]. They confirmed that nonlinear resonances are responsible for the

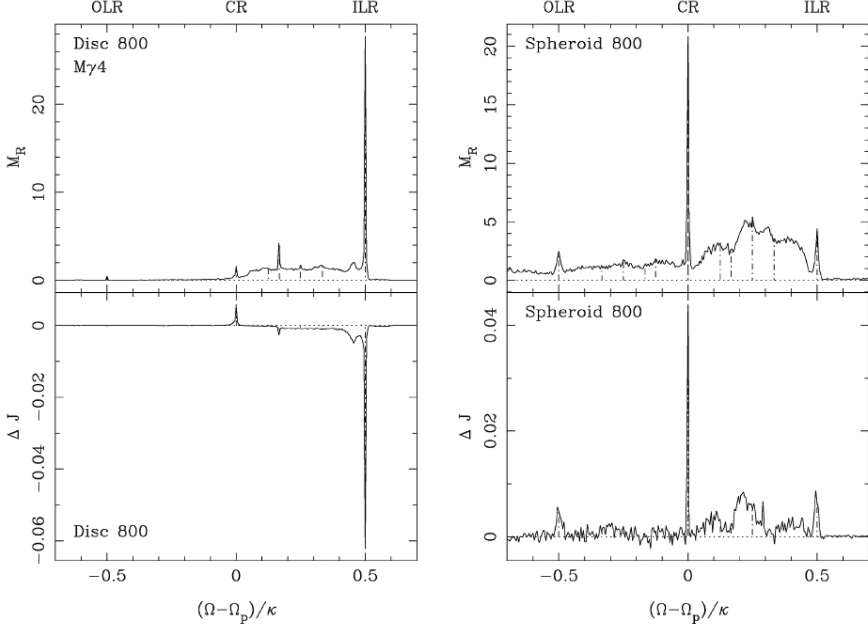


Fig. 7.4. Barred galactic disk–DM halo angular momentum transfer using resonances in numerical simulations. Upper panels: total mass of trapped particles at the resonances, M_R vs. normalized frequency $\Omega - \Omega_p/\kappa$. Lower panels: change in the angular momentum J vs. normalized frequency. The left and right panels correspond to disk and halo components, respectively. Vertical dot-dashed lines give the positions of main resonances. (From [8].)

bulk of J transfer to the halo, and that linear resonances follow this trend only roughly.

One of the most important corollaries of angular momentum transfer away from the bar region in the disk, i.e., within the CR, is the bar slowdown. This slowdown leads to an additional effect — the bar becomes stronger. The reason for this is that one can envision the bar having two types of angular momenta, the tumbling and internal (circulation). The former J determines Ω_b , while the latter one shapes the (ellipticity of) orbits trapped by the bar, i.e., ϵ . Of course, the bar cannot strengthen indefinitely — when $\epsilon \rightarrow 0.8$, the fraction of chaotic orbits within the bar grows sharply, saturating its strength. Nevertheless, a substantial slowdown of stellar bars leads to an apparent discrepancy between simulations and observations. If the bars are indeed long-lived, they are expected to slowdown and be short of the CR radius. Observations point to bars extending to the CR — the so-called fast bars. However, additional factors can delay or saturate the bar growth well below the above maximal strength, as we discuss below.

The above conclusions were based on the analysis of nonrotating DM halos. For spinning halos, [120], a new effect has been observed — ability of a DM halo to absorb J saturates, and this happens faster with the increase of the halo's

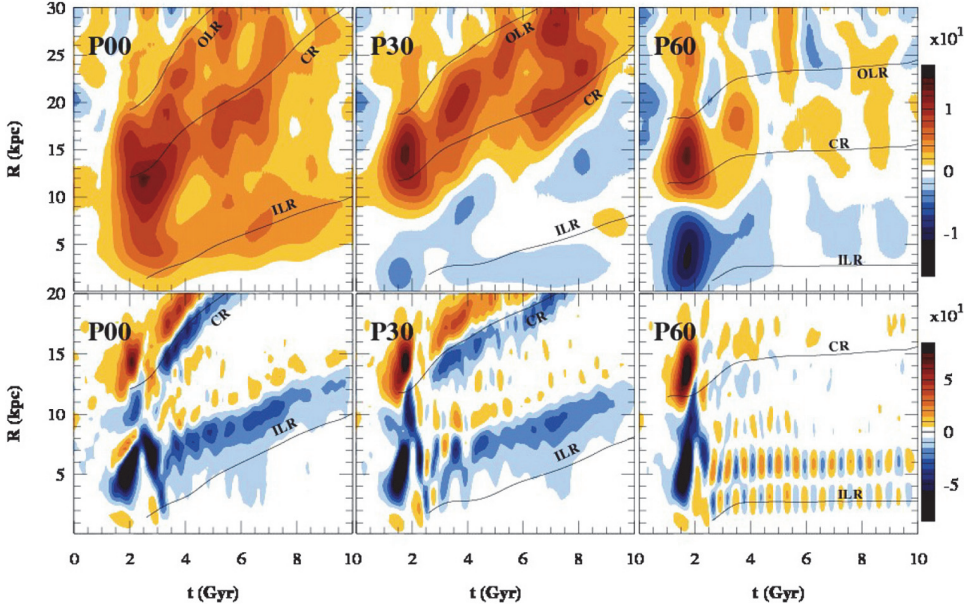


Fig. 7.5. Effect of the halo spin on J transfer from disk to DM halo: rate of angular momentum flow $\dot{J}$ as a function of the cylindrical radius R and time for three representative numerical models of spherical DM halos with a cosmological spin parameter $\lambda = 0$ (left column), 0.03 (middle column) and 0.06 (right column). The top panels correspond to the DM halo and the bottom panels to the stellar disk. The color palette uses a logarithmic scale in color, and represents the absorption/emission of J . The main resonances are indicated by the black solid lines. The cylindrical shells have $\Delta R = 0.5 \text{ kpc}$ and $z = \pm\infty$ for the halo and $|\Delta z| = 3 \text{ kpc}$ for the disk. (From [120].)

cosmological spin parameter λ . As a result, the inner halo starts to emit J which is absorbed by the bar and by the outer halo. Figure 7.5 underlines this behavior. For $\lambda = 0$, the halo only absorbs J , and so is the outer disk beyond the CR radius. At the same time, the disk emits most strongly at its ILR as well as in the UHR region, which is the 4:1 resonance. The $\lambda = 0.03$ model displays strong absorption of J at CR–ILR regions, and a mild emission by the inner halo. The disk emission appears to be largely unchanged. The $\lambda = 0.06$ model exhibits a strong emission by the inner halo and a weakened absorption by the outer halo. The disk emission of J at the ILR is very weak, and appears to be intermittent with a weak absorption. In fact, emission and absorption by the different halo regions, e.g., ILR and CR, are intermittent as well and appear anticorrelated at the same time. The halo OLR and ILR emission/absorption are correlated.

The most important corollary of this effect for the bar evolution is its strength and slowdown. Bars evolving in spinning halos have a limited growth and slowdown much less than in nonrotating halos, i.e., rate of change in the bar pattern speed, $\dot{\Omega}_b$, anticorrelates with λ . This behavior is shown in Fig. 7.6, where models with $\lambda = 0\text{--}0.09$ are shown. $\lambda = 0$ displays the typical behavior of bars in numerical

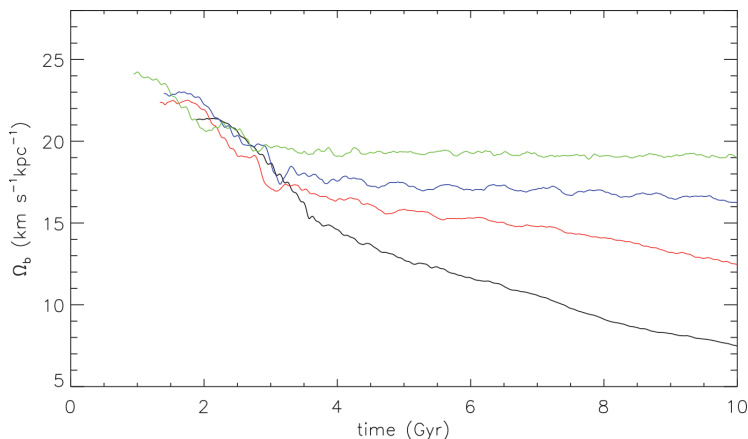


Fig. 7.6. Effect of the halo spin on the bar slowdown: evolution of bar pattern speed Ω_b for spinning spherical halos with (bottom to top) $\lambda = 0, 0.03, 0.045$, and 0.06 . (From [120].)

simulation with about a factor of 4–5 slowdown of Ω_b over few Gyrs. In contrast, $\lambda = 0.045$ pattern speed decays by about 1/3 only, and for higher λ it decays even less. The difference in the bar evolution is even more dramatic, if one emphasizes only the secular evolution, i.e., after the buckling instability in the bar (discussed below). In fact, model bars with $\lambda \gtrsim 0.05$ slowdown insignificantly over 7 Gyr. The reason for this interesting behavior of galactic bars lies in the saturation of their growth by the angular momentum pumping from the DM halos back to the disk. Remember that a fraction of J which goes into orbits that comprise the bar make them less oval, and the bar less strong.

Recurrent buckling instability in galactic bars: While bars can form as a result of a dynamical instability, they themselves are subject to instabilities, of which the most prominent one is the vertical buckling instability, first detected in numerical simulations [37]. Subsequently, it received two alternative explanations, namely, a resonant bending [38] and a firehose instability [147], see also [168, 190]. The buckling behaved as a dynamical instability — the disk flip-flopped in the central few kpc with a characteristic timescale of ~ 100 – 200 Myr which resulted in the vertical thickening of the stellar bars and a spectacular breaking of its vertical symmetry (see, e.g., Fig. 7.7). It attracted interest because it led to the formation of peanut/boxy-shaped bulges supported by rotation in the disk plane in contrast with the classical bulges supported mostly by stellar dispersion velocities. Such disky bulges with characteristic shapes have been observed in the edge-on galaxies [111], and the fraction of peanut/boxy bulges is high [123]. Moreover, simulations have shown that bars weaken as a result of this instability and it was further speculated that buckling can lead to the bar dissolution [147] — not supported by a detailed analysis of stellar orbits in the bar [132]. Furthermore, Pfenniger and Friedli [146] have identified 3D families of orbits, so-called bananas and antibananas, which,

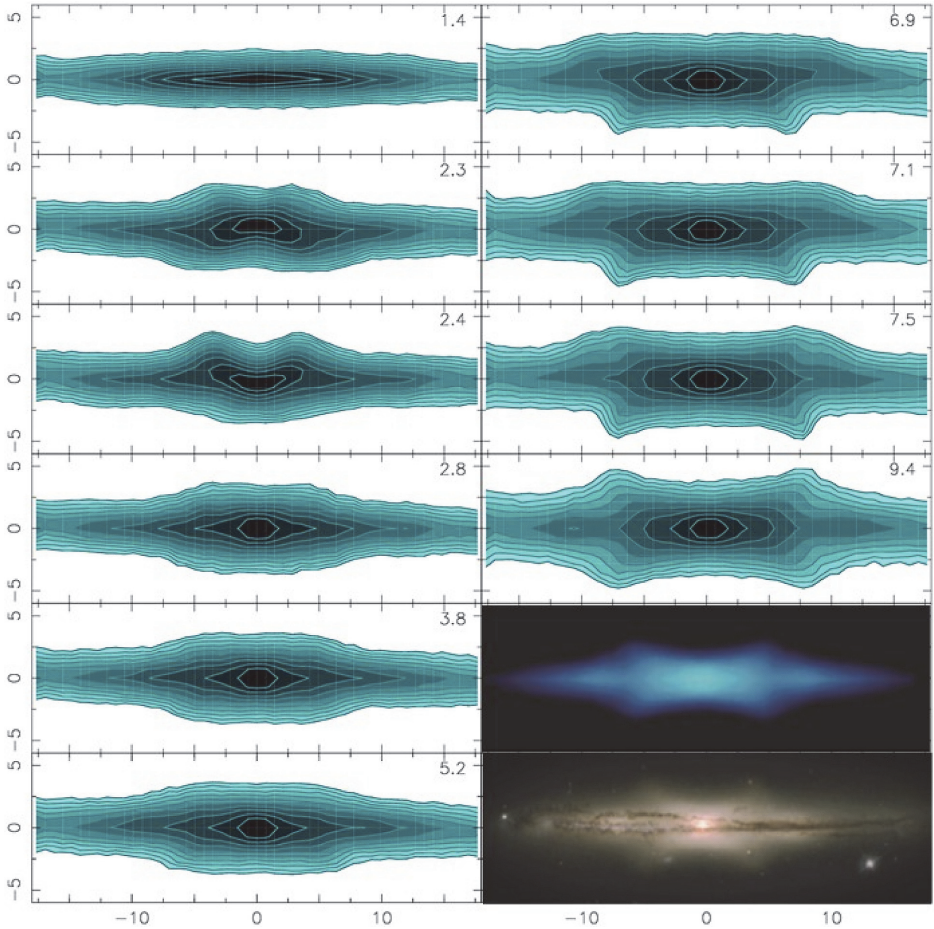


Fig. 7.7. The recurrent buckling instability in galactic bars in numerical modeling. Left and upper right frames: Evolution of the vertical structure in the bar — edge-on view along the bar minor axis. The length is given in kpc, and the values of the projected density isodensity contours are kept fixed. The time in Gyrs is given in the upper right corners. Note, the bar flip-flops at 2.3–2.4 Gyr (first buckling), and the growing/decreasing vertical asymmetry at 5.2–7.5 Gyr (second buckling). (From [133].) Low right-hand frames: smoothed version (top) of the 9.4 Gyr frame, and a matching galaxy from HCG 87 group of galaxies (bottom frame, Hubble Heritage Team), courtesy of J. H. Knapen. (See Video 4, page xiii.)

when populated, lead to the specific shapes of the central bulges, when viewed along the bar minor axis. After the dynamical asymmetric stage, the bulge acquires its boxy shape due to the higher resonances populating additional orbits.

Careful analysis of bar evolution during and after the buckling have found that this instability is *recurrent*, and exhibits a secular behavior after the first dynamical phase [133]. Figure 7.7 provides an example of the second stage of buckling instability, which is triggered around 5 Gyr and is observable till ~ 9 Gyr. Unlike the first

stage, this stage proceeds via the outer part of the bar, where the “peanuts” become much more pronounced, even X-shaped, and profoundly asymmetric. However, not all bars experience recurrent buckling, and the reason for this is not yet clear.

7.5.1.3. *Dark matter halo bar*

Some mass redistribution in the parent DM halo can be observed as well in response to the stellar bar. This so-called DM bar, or “ghost” bar, is clearly triggered by the underlying stellar bar, and is much weaker [41]. A simple numerical experiment in dispersing the stellar bar, by redistributing the stars azimuthally, also leads to an immediate dissolution of the DM bar (see [180] which is based on [16]). The DM particles trapped in the ghost bar appear to be those near the halo ILR [8].

7.5.1.4. *Stellar bars with gas*

Addition of the gas component to the barred disk leads to a substantially more pronounced response — gas orbits shock when crossing. First simulations of bar-driven shocks in galactic disks have explained many of the observed features [98], such as an existence and shapes of the dust lanes within the bars [5], formation of resonance rings [81, 110, 165], nuclear spirals [64], etc.

Most importantly, the gas experiences a delayed response to gravitational torquing from the stellar bars, shocks and streams inwards, accumulating within the ILR, or within the OILR, if two resonances exist. In this latter case, the torques are reverses inside the IILR and move the gas out across this resonance. Hence, two resonant rings form in this region. Subsequently, they interact and merge [81–83, 110]. Additional resonance rings form at the UHR and OLR, as is frequently observed in barred galaxies.

The resonant ring formation is due to the gas which accumulates there. This gaseous ring perturbs the underlying gravitational potential and skews the main orbits supporting the bar. Active SF confirms the fresh gas supply to the rings, which is both observed in the multiwavelength observations [99, 109] and reproduced in numerical simulations [81, 99, 110]. Fossil stellar rings can exist for a long time after the gas flow ceased to support the SF there [178].

7.5.1.5. *Nested bars: Dissipative and non-dissipative dynamics*

Double-barred systems show a complex dynamical behavior resulting from gravitational quadrupoles of both bars “talking” to each other. Mutual interactions of nested bars can lead either to chaotic response of stellar and gas orbits, or to coupling between the bars [65, 82, 83, 128, 129, 174, 179]. Nested bars consist of stellar large-scale and nuclear bars, of a few kpc and $\lesssim 1$ kpc, respectively. Quite unexpectedly, about one-third of all barred disks host additional nuclear bar [66, 67, 114], these must be long-lived systems. Nuclear bars almost always come in conjunction with large-scale bars [114]. This is a clear indication that the later ones

are a prerequisite for their formation, and hence called primary, while their small counterparts are called secondary. It is possible, in principle, to envisage a scenario where they form separately, although the necessary conditions for this appear artificial. Claims to the contrary misinterpret the initial conditions. Finally, most of the detected nuclear bars are star-dominated. Comparable statistics of gas-dominated bars are unavailable at present. Observational properties of nuclear bars have been summarized in [179].

What makes the nested bars truly unique is their ability to couple and decouple. To avoid confusion in terminology here, we note that nested bars are always coupled dynamically, i.e., they are in the state of mutual dynamical interaction. Additional parameter that can describe them is Ω_s/Ω_p — the ratio of secondary-to-primary bar pattern speeds, which can be unity, integer, or any number. We describe the system as being coupled when $\Omega_s/\Omega_p = 1$, i.e., the bars corotate; being partially “decoupled” when the CR of the secondary coincides with the ILR of the primary, thus reducing the chaos in the system; and being in a completely “decoupled” state when Ω_s/Ω_p is arbitrary, and so the system is in the transient state. While the first two states mentioned can live indefinitely long, the transient is limited in time. In this respect, the nested bars are the astrophysical counterpart of coupled nonlinear oscillators [118]. Numerical simulations have demonstrated that in the process of evolution, nested bars form with $\Omega_s/\Omega_p = 1$, and that dissipation is necessary to switch the state to $\Omega_s/\Omega_p > 1$ [65, 74, 110].

Resonances are very important in linear and nonlinear dynamics. Typically, they increase dissipation in the gas. A less trivial is the purely nonlinear effect of the mode coupling [187]. The basic idea is that nonlinear modes can exchange energies and angular momenta, and hence provide self-regulation to pattern speeds, which otherwise would decay with time. The details of the mode coupling in triggering the partially coupled nested bars remain obscure.

For pure stellar nested bars, the decoupling is achieved through initial conditions only and the nested bar state is long-lived in models with a sufficient mass resolution [74, 179]. Limits of mass ratios of nested bars exist, with the majority of regular stellar trajectories confined to each bar [59]. Moreover, multiple-periodic orbits, called loops, have been found, which form the backbone gravitational potential in such systems [128].

Gas-dominated nuclear bars: Large-scale bars channel the gas toward the central kpc, as we have discussed above. Under various conditions, such as the strength of the ILR, the gas can either accumulate in the nuclear rings, or, if its self-gravity is sufficient, experience a runaway collapse, typically in the form of a gaseous nuclear bar [65, 74, 110, 174, 175]. Dynamical importance of the gas can be increased if its mass fraction exceeds $\sim 10\%$ within the central kpc. Random velocities in the gas are typically lower than stellar dispersion velocities. During the decoupling process, the gaseous bar develops and strengthens. This leads to the increased population of chaotic orbits [132, 188]. Under similar circumstances, this would dissolve or

weaken a stellar bar. But gas cannot be retained on intersecting chaotic orbits. It shocks, which results in the avalanche collapse on the center, which is related to the self-organized criticality [118]. In this process, the gaseous bar speeds up and contracts.

Gas inflows in nuclear bars which are dominated by stars, can be recurrent, and will depend on the external fuel supply. Such nested bars can exist for a long time without any gas transfer. During fueling periods, the star formation efficiency can be severely inhibited because of a large shear and developed turbulence [83]. Therefore, nuclear bars are expected to contain an older stellar population, with some admixture of younger stars, but without any ongoing star formation, as indeed has been observed (see, e.g., [48, 75]), and supported by numerical simulations. An important conclusion is that stellar population age in nuclear bars is not related directly to their ability of fueling central activity in disk galaxies. Whether these inflows can extend and fuel the central SMBH in active galaxies is to be seen.

7.5.2. *Feedback*

Feedback is defined as a cause-and-response chain of events that forms a causal stable or unstable loop. In the former case, the process is self-regulating, and the feedback is negative. In the latter case, the system is obliged to find a new stable loop or to disintegrate, meaning that the feedback is positive. Positive or negative feedback during disk evolution can change the star formation rate (SFR). The list of relevant processes contributing to feedback is a long one — stellar and AGN radiation, winds (stellar, AGN, galactic), AGN jets and their cocoons, turbulence, supernovae (SN), their bubbles and superbubbles, spiral density waves, stellar/gaseous bars, and cold accretion from the cosmological filaments (to be discussed below). Fully understanding the disk response to the above processes is decisive for predicting the feedback loop. The physics of AGN feedback is not fully understood at present, and our description of turbulence remains rather empirical. Both turbulence and star formation are below the resolution level of current numerical models, and are treated at the subgrid level, i.e., purely phenomenologically.

7.5.2.1. *Feedback and star formation*

The fraction of baryons converted into stars over the Hubble time is very small. The underlying reason for this must be various processes which lower the conversion efficiency and which must be accounted for in order to understand the cosmological evolution of galaxies. For example, numerical simulations have demonstrated that energy, momentum, and mass deposition by stars and AGN have a profound effect on the state of the star forming gas [151, 162]. Without this feedback, there is an overproduction of metals, especially in small galaxies, and the gas overcooling becomes a problem [131].

Models with a weak feedback appear to overproduce the baryonic masses of galaxies, especially for the most and least massive objects [106]. Various attempted

models for the feedback, such as AGN “radio mode”, did not improve the situation. In a way, the AGN is treated as a giant O star at present. The overall conclusion is that more “sophisticated” feedback models are necessary to solve the problem.

Galaxy morphology can provide a testing ground for understanding various feedback mechanisms. For example, an unexpectedly large fraction, $\sim 70\%$, of massive $\gtrsim 10^{10} M_\odot$ galactic disks have bulge-to-total mass ratio, B/T , of $\lesssim 0.2$, both in barred and unbarred galaxies [71, 201]. This result is in a stark contrast by more than an order of magnitude with predictions from numerical modeling — only disks that did not experience major mergers since $z \sim 2$ are expected to have such low B/T . It also raises a question about the role of mergers in the formation of galactic bulges. While mergers can contribute to the formation of classical bulges supported mainly by stellar dispersion velocities, the disk bulges (see [111]) can form as a result of buckling instabilities in galactic bars, as discussed in Section 7.5.1.

Gravitational feedback involves collisional heating during mergers. Shocks help to virialize gas — a process whose efficiency depends on the orbits of merger components, affecting most the low-density gas in the outer parts of galaxies. Most of this gas remains bound to the merger product.

Gas pressure gradient (i.e., thermal) feedback depends on the ability of the ISM to build a high pressure bubble, which either expands in 3D or forms a de Laval nozzle. The energy source for the bubble can come from SNe, AGN input, etc.

SN feedback is the most analyzed one in the literature (for a review, see, e.g., [179]). Kinetic energies of SNe II and Ia are similar, but the latter one is deposited away from the star forming regions. Estimates show that the gas can be removed from DM halos having virial velocities of $\lesssim 100 \text{ km s}^{-1}$ when a substantial fraction of gas is converted into stars, say $M_* \sim M_{\text{gas}}$. The related DM virial mass is $\sim 2 \times 10^{11} M_\odot$ and $M_* \sim 3\text{--}4 \times 10^{10} M_\odot$ [44]. This is in agreement with the characteristic mass for a bimodal evolution mentioned in Section 7.6.

The ISM can be reheated by the SN feedback and pushed into the halo, and its large fraction expelled from small galaxies. If a large fraction of the original gas has been converted into stars, the rest of the gas can be driven out of a galaxy by the SN feedback. However, the efficiency of converting the stellar mass into kinetic energy by the SNe, $f_{\text{SN}} \equiv \epsilon/100 M_\odot c^2 \sim 3 \times 10^{-6}$, is low. Here, $\epsilon \sim 10^{51} \text{ erg}$ is the initial energy released by a typical SN. While substantial progress has been made in high-resolution numerical simulations of SN shells sweeping up the ISM, much of the detailed evolution is not clear yet. In particular, how efficiently is this energy distributed among the baryons must be studied.

OB stellar winds are known to be driven by radiation pressure in the resonance lines of the CNO elements. Overall, these winds inject a comparable amount of kinetic energy over their lifetime to the SNe. The typical velocities of these winds are $\sim 2\text{--}3 \times 10^3 \text{ km s}^{-1}$. These winds have been incorporated into numerical simulations at the subgrid level [80, 110]. Understanding the development and the

overall effect of galactic winds driven by a combined action of OB stars and SNe is complicated and remains an unresolved problem.

AGN feedback: The origin of AGN winds and jets lies within a fraction of a pc to few 100 pc from the SMBH. They can be driven by energy and/or momentum input from various processes in the region. We limit our discussion to subrelativistic AGN winds, and exclude the jets. Two main classes of outflows exist: hydromagnetically-driven (MHD) and radiation-driven from the underlying accretion disks. The MHD winds have been worked out by Blandford and Payne [21] for a specific density law, and generalized by Emmering *et al.* [63]. These winds feed on the rotational energy in the disk. Other models of MHD winds have been proposed [122].

Radiation-driven winds from AGN disks are driven by absorption (scattering) in the resonance lines of the CNO elements [173], similar to those in OB stars, and by dust. MHD winds are much more efficient in extracting the angular momentum from accretion flows compared to the radiation-driven winds. They are able to reduce the mass accretion rate substantially, or even make mass outflow rate larger than accretion. On the other hand, the MHD winds can extract angular momentum without much of the outflow at all, which is in completely contrast to the ability of radiation-driven winds. A rough estimate of the AGN feedback efficiency analogous to the SNe is $f_{\text{AGN}} \sim 10^{-4}\eta$, where $\eta \sim 10^{-3} - 1$ is the conversion factor of AGN bolometric luminosity into mechanical luminosity [181].

To account for the AGN feedback in high-resolution simulations was first attempted by invoking pure thermal feedback [183]. It has been assumed that a fraction of isotropic bolometric AGN luminosity has been deposited locally. Momentum transfer was not accounted for. Resulting feedback has limited the growth of the SMBH and expulsion of the ISM from the galaxy. More detailed followup simulations have shown that momentum transfer dominates over energy deposition because of the short cooling timescales and the inability to retain thermal energy in the dense gas located in the central region of galaxies [143]. The same is symptomatic of stellar winds and disk winds with effective temperatures in the UV.

Clearly, AGN winds can have a dramatic effect on the ISM and intergalactic medium (IGM) if one can ensure their efficient coupling with baryons, for example, if this energy, momentum, and mass loss around from the SMBHs were distributed in a highly symmetric fashion. However, how exactly this coupling with baryons is achieved is still unknown. Even when the feedback energy exceeds the gas binding energy, it can escape along the preferred directions, and involve fluidized bed-type phase transition, dramatically reducing the feedback. Models proposed so far based on energy- and momentum-driven outflows are mostly phenomenological.

Galactic winds: Presently, almost any wind model experiences difficulties from any object, stellar, or accretion disk. Clearly, however, such winds are ubiquitous (e.g., see the review in [79]). Mostly, they are driven by SNe and winds from OB stars. The contribution of AGN is still unclear. The driving by the SNe and OB stars forms a bubble of $\sim 10^{7-8}$ K gas, which expands down the steepest pressure

gradient and enters the “blowout” stage. This is probably the main way that highly enriched material can be injected into the halo and the IGM. The winds appear inhomogeneous and carry embedded $\sim 10^4$ K clouds, so represent a multiphase ISM.

To circumvent the lack of numerical resolution, the necessary physics (when known) can be introduced at the subgrid level. Four representative models are given below.

- (1) **Constant wind model** [182] has introduced the multiphase ISM. Two phases, cold and hot, coexist in a single smoothed particle hydrodynamics (SPH), and cannot be separated dynamically. The two phases are followed when the density is above the critical gas density threshold, ρ_{SF} . Above this threshold, the star formation is allowed to proceed. The SNe modify equation of state and heat the ambient hot phase with a long cooling timescale. Thermal conduction from the hot phase heats up and evaporates the cold phase. Mass-exchange equations between the phases are solved analytically. The galactic winds are triggered by converting the dynamics of some gas particles into “wind” particles. The latter are not subject to hydrodynamical forces, and experience the initial kick from the SN. All wind particles have the same velocity and the same mass-loading factor $\beta_w \equiv \dot{M}_w / \dot{M}_{\text{SF}}$, where $\dot{M}_w$ and $\dot{M}_{\text{SF}}$ are the wind mass loss rate and the star formation rate (SFR), respectively.
- (2) **Delayed cooling wind model** [85, 189]. A fixed number of neighboring SPH particles, whose cooling is disabled, are affected by the energy injection from the SN and OB stellar winds. Such a process is resolved by at least five time-steps, and extends to $t_{\text{in}} \sim 3 \times 10^7$ yr, which represents the feedback timescale. The SN energy is deposited in the thermal energy and converted into the kinetic energy using equation of motion and the energy thermalization parameter. The affected particles are not subject to hydrodynamical forces for a time period which depends on the minimum of t_{in} and the time it takes the particle to cross into a region with density below a prescribed threshold.
- (3) **Blastwave wind model** [186] is based on the adiabatic (Sedov–Taylor) and snowplow phases in the SN expansion. The blastwave is triggered by a combined action of many Type II SNe. The maximum radius of the blastwave, R_{blast} , is obtained phenomenologically [33, 135], and radiative cooling is disabled for radii smaller than R_{blast} .
- (4) **Variable wind model** [34] adopts a subgrid multiphase ISM. Wind particles are selected based on density and temperature criteria. The main parameters are the wind mass load β_w , defined above, and the wind velocity v_w constrained observationally and computed on-the-fly. These parameters are expressed in terms of host galaxy stellar mass M_* and the SFR. The threshold density for SF, ρ_{SF} , is based on the surface density of the Kennicutt–Schmidt law. The wind velocity is calculated as a fraction of the escape speed from the host DM halo, and is parameterized as momentum- or energy-driven wind. It is an increasing function of the redshift and the SFR.

7.6. Externally-driven evolution in disk galaxies

Early models of galaxy formation considered them being essentially isolated systems forming as a result of a gravitational collapse (see, e.g., [55, 149]) within DM halos [202], leading to the formation of galactic disks [69]. A complementary view that galaxy interactions and mergers are a direct corollary of structure formation and drive galaxy evolution in the universe has been promoted as well [192]. In order to grow, galaxies and their host DM halos should rely on the external reservoir of baryons and DM. Numerical simulations have allowed a quantitative study of external drivers in secular evolution in disk galaxies: mergers and accretion from cosmological filaments.

Major mergers, defined at mass ratios from 1:1 to 1:3, have strong effect on stellar disks, down to their complete destruction and transformation into spheroidal component. As this happens as fast as on one to few crossing times, these mergers drive dynamical rather than secular evolution. Intermediate and minor mergers, with mass ratios of 1:4 to 1:10, and below, respectively, have lower amplitude dynamical effects, but, because they are much more frequent, relentlessly drive mass and angular momentum redistribution in the disk. At the very end of this mass ratio, one can define “smooth” mass accretion of unprocessed gas by stars as well as DM. New results have successfully challenged the merger-dominated scenario of the galaxy growth — the new paradigm is focused on the galaxy growth by smooth accretion from cosmological filaments (see, e.g., [45, 46, 70, 105, 106, 181]).

7.6.1. Galaxy growth by mergers

Mergers appear to represent a diverse phenomenon and their products are equally diverse. Mergers can be defined as an encounter of two or more galaxies, which results in the formation of a single galaxy. The importance of mergers should grow with redshift, $\propto (1+z)^m$, although the observed rate exhibits a substantial scatter. Extending observations to fainter magnitudes generally shows an increase in m . Differences exist between measured rates for rich clusters ($m = 6 \pm 2$ [196]) and field galaxies ($m = 2.7 \pm 0.6$ [115]), and when using different methods, such as close pairs and morphology. A substantial difference in the major merger rates of $m = 3.43 \pm 0.49$ and 2.18 ± 0.18 has emerged from a comparison between NIR and optical bands [148]. Finally, diverse observations have resulted in $m = 2 \pm 2$. At the same time, numerical simulations have indicated a narrow range of $m \sim 3$, while ignoring the possibility of multiple galaxies per DM halo.

Dynamical friction: Mergers can occur also from unbound orbits. Only galaxies with relative velocities less than their internal dispersion velocities, $v_{\text{rel}} \lesssim \sigma$, will merge, as a rule of thumb. Within large galaxies, $\sigma \sim 200\text{--}300 \text{ km s}^{-1}$, while that of the clusters of galaxies $\sim 500\text{--}1000 \text{ km s}^{-1}$. The merger orbital angular momentum J , depends, on v_{rel} , but this dependence is short-lived — the halo J or cosmological spin, λ , experiences a sharp increase during a major merger, but subsequent mass

and energy redistribution in the halo washes out the gain [89, 153]. The corollary is that there is no steady increase in λ with time due to major mergers. A simple prescription to increase the parameter space available to mergers is to invoke dynamical friction process.

The DM appears to be an important contributor to dynamical friction. For circular orbits, analytical solution is possible. However, more realistically, the galaxy dives along a very elongated orbit, with a small pericenter. This leads to a tidal disruption, supplemented by a mass loss very early in the process. The analytical solution becomes more complicated, and decreases the characteristic timescale for the friction [23, 50], as confirmed in numerical simulations [157]. Corollary, which becomes most interesting, is the importance of resonances between the orbital motion and stellar motions in the disk (if it is present). These are absent in Chandrasekhar's original formalism. We do not list additional intricacies here, which are discussed elsewhere [138].

Phase mixing and violent relaxation: The two-body relaxation timescale is way too long to have an effect on mergers dominated by collisionless processes — phase mixing and violent relaxation [124]. The idea of phase mixing invokes the evolution of a coarse-grained distribution function in a collisionless system. The fine-grained function is time-independent because the classical entropy is conserved, while coarse-grained function evolves to uniformly cover the available phase space for the system, maximizing the coarse-grained entropy. Hence, phase mixing destroys an organized phase-space structure.

Nonconservation of the particle specific energy leads to a violent relaxation which proceeds in the time-dependent potential. It establishes the Maxwellian distribution of velocities, when a temperature is proportional to the particle mass. So, dispersion velocities of the particles are independent of mass of the particles. Violent relaxation is most relevant during the system virialization, and the characteristic timescale is the system crossing time. The process is most complete in the central regions, but galaxy interactions will contribute most in the outer regions. Overall, the efficiency of the process is unclear.

Mergers wet and dry: Mergers including systems of stars and DM are called dry mergers. Limited observational data exist on them, mostly in clusters of galaxies [196]. The end product of these mergers is expected to be an elliptical system [11, 191]. The formation of the red sequence of massive galaxies can be related to dry mergers for $z \lesssim 1$, because of insufficient amount of massive blue galaxies [68, 107].

Multiple dry mergers preserve the Faber–Jackson relation, as shown by N -body simulations. But the latter produce lower central dispersion velocities and increase the effective radius. The fundamental plane of ellipticals remains thin. So fundamental scaling relations are robust against dry merging. It remains, however, unclear when these relations are established.

Wet mergers are dissipative. When galactic disks are involved, the outcome is determined by many parameters, such as disk inclination with respect to the orbital plane, and the alignment of internal and orbital spins, i.e., prograde vs. retrograde encounters. The first modeling of disk interactions was performed using a light-bulb “supercomputer” [91]. Modern simulations address a long list of physical processes in interacting galaxies, i.e., stretching, harassment, stripping, strangulation, squelching, threshing, splashback, and cannibalism [138]. They also attempt to include effects on the SFRs, and quenching the SF.

7.6.1.1. *Mergers products: Disks and spheroids*

The result of disk galaxy mergers can be either disk or spheroid. Early deliberations on disk merger remnants were based on models without or with low-resolution gas. The DM halos have been “soaking up” the internal and orbital angular momenta of merging galaxies, and collisions appeared sticky [86]. The dynamical role of gas has been shown to exceed its mass fraction in isolated and cosmological models [12, 80, 176]. Gas also shortens the merging timescale [12]. Simulations of disks with $\lesssim 10\%$ led to the formation of spheroidal stellar component with the de Vaucouleurs $1/4$ law surface brightness, supplemented by the central cusp which is not observed in such galaxies. They have also shown that the formation of some ellipticals can be related to the wet mergers. But what fraction of ellipticals has formed this way?

The scenario of ellipticals forming in a binary major mergers of disks experiences the following difficulties: typical ellipticals are more metal-rich than present-day disks, their stellar populations are older and seem to form on shorter timescales, binary mergers of present-day disks could not lead to massive ellipticals (but could form from high- z disks), binary mergers of any kind are not isotropic, while massive ellipticals are.

An important question is whether disks can survive mergers, especially major mergers. In the absence of gas, simulations of disk mergers show a clear trend of thickening and destroying disks [152]. But what if the disk contains gas and there are plenty of “leftovers” from mergers? What is the critical fraction f_{gas} for the survival of a disk?

Simulations have demonstrated that after some major mergers the disks can reform, if enough gas can be maintained, for example, in simulations of pure gas, bulgeless disks on prograde parabolic orbits, in the presence of SF [184], and for gas-rich disks with $f_{\text{gas}} \gtrsim 0.5$ [152]. Another example of disk rebuilding has been simulation of 1.6:1 wet merger at $z \sim 0.8$ [77], using blastwave approximation discussed earlier. For $z < 3$, the disk $f_{\text{gas}} < 0.25$. The disk has been rebuilt over a few Gyrs, and the old stellar population in the thick disk has faded away, while the thin disk dominated in the I -band.

Also, recent high-resolution simulations have shown that disk heating has been overestimated in minor mergers [92, 155], and that a resilient, disk-dominated population of galaxies forms [158]. A follow-up analysis of evolving disks reveals that

the dominant growth mode is rather via accretion of cold gas [159] and not via mergers, as discussed in Section 7.6.2.

Clearly, a number of far-reaching conclusions follow attempts to rebuild and sustain disks over cosmological times. First, the existence of a thick stellar disk component is required, representing the population of a pre-merger disk. Second, it takes a few Gyrs to rebuild the disks at low z , and it is encouraging that at $z \gtrsim 6$ this timescale is shorter by about a factor of ten, and the morphology-density correlation maintained during the reionization does not follow the trend it displays at low z [158]. Third, the observed frequency and mass fraction of classical bulges in disk galaxies are debatable at present with respect to other bulge types. The origin of the disk bulges (Section 7.5.1) is apparently unrelated to galaxy interactions, but results from the buckling instabilities of stellar bars [14, 38, 111, 133, 144, 147]. Because simulations depend on the subgrid (and sometimes unknown) physics, attempts have focused on semianalytical models, although their predictive power has not been verified.

Attempts to predict properties of merger remnants and to quantify the contribution of classical bulge formation from mergers of various mass ratios have been made using observational constraints on disk masses and gas fractions in galaxies. The main conclusion was that the assembly of L_* bulges is dominated by major mergers, while bulge formation in the low-mass systems is determined by minor mergers. The merger mass ratio, μ_{gal} , was found to be traced by the ratio B/T . Moreover, correlation $B/T \sim \mu_{\text{gal}}(1 - f_{\text{gas}})$ has been identified. Taking at the face value, this means that increasing f_{gas} tends to suppress the bulge formation. In other words, it can be interpreted in terms of a reduced efficiency of gas angular momentum loss with increasing f_{gas} . The byproduct of this conclusion is that collisionless systems lose angular momentum more efficiently than the dissipative ones. This is difficult to accept.

7.6.2. *Accretion from cosmological filaments*

In terms of mass growth, what is the main contributor to galaxies? Taking the simplistic approach of the mass ratio sequence discussed above, what is the role of the low-mass tail in the merger-driven evolution? How do galaxies get their gas? After all, the fresh gas supply is essential in order to fuel the SF in the disk. This gas should have sufficiently low temperature to be retained by the disk, e.g., $\lesssim 10^5$ K. Alternatively, higher $T \sim 10^6$ K gas, of the order of the halo virial temperature, should be able to cool down on a short enough timescale, at least over few Gyrs. Similarly important appears to be the anisotropic accretion along the cosmological filaments in contrast with the spherical or axisymmetric accretion in the context of isolated models. Finally, cold gas tends to clump. Accretion shock which can virialize the gas by heating it up will have an opposite effect on clumpy gas than on the uniform one — such gas would be rather compressed and able to cool than heated up.

While the frequency of galaxy mergers increases steeply with redshift, the availability of an unvirialized gas increases as well. The capability of galaxies to grow via accretion has been known for some time. It has been assumed that gas falling into DM halo experiences shocks and heats up to a virial temperature, T_{vir} , in the vicinity of the virial radius and fills it, remaining in a quasi-hydrostatic equilibrium with $T_{\text{vir}} \sim 10^6 (v_{\text{circ}}/167 \text{ km s}^{-1})^2 \text{ K}$. Such a hot gas cools from the center out, loses the pressure support and settles into a disk-supported centrifugally [69, 149, 202].

This point of view has been successfully challenged now in that some of the gas avoids being shocked when entering the halo. For example, gas is capable of entering the halo along dense filaments, penetrating deeply.

A simple one-dimensional (1D) model of gas accretion in a spherical DM halo has shown that a critical value for the halo mass exists above which the shock is supported at the virial radius [20]. It depends weakly on the redshift of halo virialization and strongly on gas metallicity, as it affects the cooling rate significantly. The characteristic halo mass is $\sim 10^{11} M_{\odot}$, has a primordial gas composition, and $\sim 5 \times 10^{11} M_{\odot}$ for about 0.05 of the solar metallicity. For this metallicity, the Press–Schechter halos will generate stable shocks only by $z \sim 1.6$. The consequence is that stable shocks will form only in massive halos and at low redshifts. The necessary condition for the shock stability is that the cooling timescale of the shocked gas should be longer than the compression timescale. However, the 1D hydrodynamics cannot capture additional solutions which depend on geometry. In particular, it is possible that the inflow would join the disk inside the halo smoothly without being shock-heated.

A number of additional issues can complicate the above conclusions based on 1D: triaxial halos shapes with arbitrary axial ratios, interactions between the forming disk and the supersonic gas infall, and the plausible trapping within the halo gas of Ly α photons.

Numerical simulations have addressed a number of issues, such as what is the maximum temperature of gas entering the halos. The standard view was that $T_{\text{max}} \sim T_{\text{vir}}$. Is all the gas shocked when entering the halo? It is constructive to define specific modes of accretion: first, a mode with a maximum temperature $T_{\text{max}} < T_{\text{vir}}$ — the cold mode, which is not shock-heated and is distributed anisotropically. Second, a hot mode with $T_{\text{max}} > T_{\text{vir}}$, which is shock-heated at the virial radius, enters a quasi-static state, cools down and is accreted quasi-isotropically. The inflow along the filaments of the cold gas has a much lower entropy, $\propto T/\rho^{2/3}$, in comparison with the shocked gas [139].

Simulations also exhibit a more complicated picture with gas accretion via filaments and by cooling of the hot halo gas [45, 105]. About half of the gas follows the anticipated path of accretion, shocks and is heated to T_{vir} . It cools down and enters the SF cycle. Remaining gas stays much cooler and bypasses the shocks. More precisely, the cold accretion dominates in low-mass galaxies and DM halos, $M_{\text{gal}} \lesssim 2 \times 10^{10} M_{\odot}$ and $M_{\text{halo}} \lesssim 2.5 \times 10^{11} M_{\odot}$. The hot accretion mode dominates

in the more massive objects. Hence, the cold accretion is expected to dominate at high z and in the low-density environment at low z . The hot accretion mode is expected to dominate in the high-density environment at low z , for example, in galaxy clusters.

The critical mass of baryons, $M_{\text{gal}} \sim 2 \times 10^{10} M_{\odot}$, determined from numerical modeling lies in the proximity to the observed characteristic mass for a shift in galaxy properties, $M_{\text{gal}} \sim 3 \times 10^{10} M_{\odot}$. This result is based on a complete sample of SDSS galaxies [104]. For stellar masses above the critical M_{gal} , no dependence on environmental factors has been found for distributions of sizes and concentrations at fixed stellar mass. On the other hand, less massive galaxies appear to follow the trend to be somewhat more concentrated and more compact in dense regions. The SF has shown much more dependence on the environment. The drop in the SFR for galaxies less massive than $\sim 3 \times 10^{10} M_{\odot}$ is ~ 10 over the density interval used in the study, which is much stronger when compared with the more massive galaxies.

So, a compelling observational evidence exists that galaxies below the critical mass show much more activity in SF, exhibit larger gas fractions, lower surface densities, and display late-type morphologies. More massive galaxies have older stellar populations, low gas fractions, higher surface densities, and early Hubble types. This *bimodal* behavior can be explained if the growth of galaxies is limited.

Cold accretion flows are yet to be detected in direct observations, although it is important to mention the already detected accretion of cold patchy gas. Because of various reasons, including low emissivity, absorption against bright sources, such as QSOs, is the most promising way to detect the cold accreting gas, especially in Ly α . High-velocity clouds around the Milky Way galaxy can be closely related to the cold accretion phenomenon.

The concurrence of cold and hot modes of accretion has a direct effect on the galaxy growth, because they depend differently on the environment, as well as on feedback from stellar evolution and AGN. They maybe also associated with different stellar initial mass functions (IMFs). Cosmic SFR shows a broad maximum at $z \gtrsim 1$ and a steep decline thereafter [130]. This decay can be associated with the decrease of the cold accretion flows [45, 105].

On the face value, below $z \sim 2$, massive $\sim 10^{12} M_{\odot}$ become typical, the shock stabilizes around halo virial radius, and the cooling time of the shocked gas becomes too long, effectively quenching the cold mode accretion. This defines the critical redshift below which the SF will be suppressed, especially in clusters of galaxies. Hence, the observed bimodality finds a logical explanation. This shutdown will result in a quick transformation of galaxies, when viewed in terms of prevailing colors of stellar populations, determined by stellar ages and the SFRs. In this case, the formation of red sequence can be tracked to the switching of prevailing accretion mode. It would provide a strong argument in favor of this scenario if a number of correlations, such as color-magnitude, bulge-to-disk mass ratio, or morphology-density, can be explained in terms of gas supply shutdown at various z and environments. However,

a caveat exists: the bulge-to-disk ratio can be affected and even dominated strongly by other processes, as has been shown explicitly [38, 133, 147].

Numerical simulations have shown that cold accretion dominates the mass supply to galaxies at $z \gtrsim 1$. At lower redshifts, the cold accretion gas decreases sharply, especially for smaller galaxies [106], which has been confirmed [26] — for galaxies up to L^* the cold accretion fuels the SF. Furthermore, high-resolution numerical simulations have detailed that the cumulative contribution of all mergers, down to 1:10, falls below that of the cold accretion, both in high and ordinary density regions [159]. In the former, the contribution of mergers is only about 10% of the smooth accretion, while in the latter it is below 20%. Moreover, the contribution to the stellar mass from mergers, is below that of the *in situ* SF. The central disk can also interact with DM subhalos, and such interactions, especially at low redshifts, can ablate the cold disk gas and quench the SF there [155].

In summary, numerical simulations of galaxy evolution have shown that galaxies develop mostly via cold and unshocked gas, while the contribution of the hot accretion mode is not important. This is a dramatic turnabout and a paradigm shift with respect to the standard picture of galaxy evolution.

7.6.2.1. Cold flows inside DM halos

For the full understanding of growth of galactic disks, one is required to analyze kinematics and dynamics of the cold flow penetrating the virial radii of DM halos and is not shocked to virial temperatures. Unfortunately, very high resolution as well as a knowledge of how various hydrodynamical instabilities operate under these conditions is necessary. How much of this cold inflow which avoids the virial shock can actually join the central disk smoothly? A number of factors play an important role in this process. First, what is the efficiency of ablation of cold streams that penetrated DM halos? Second is the evolution of the angular momentum, and third is the shape of the background gravitational potential dominated by the DM. The first factor can determine the mass influx in the cold phase — Kelvin–Helmholtz instability will lead to mixing in the surface layer of the stream. It is, however, not clear whether the mixed material will be quickly heated up due to thermal conductivity, or form a two-phase, cold-hot ISM. On top of this, the remaining mass inflow trajectory will be affected by the “friction” against the hot virialized component. Of course at high z , the hot component can be insignificant or even absent completely, as discussed earlier. The last two factors will determine trajectories of cold streams and, to a certain degree, dissipation in the infalling gas. In the cold stream gas, about 1/3 of the gas mass has been found in clumps, and the deep penetration happened even in DM halos of $\gtrsim 10^{12} M_\odot$ [46].

Most of the cosmological simulations have inadequate resolution to probe the inflow-disk interface. But it has been shown that cold gas streams can smoothly join the outer disk, being deflected from the disk rotation axis by the centrifugal barrier, and no standing shock has been detected [85]. In this case, the kinetic energy of

the infalling gas is converted into rotational energy, and the cold streams form the “cat’s cradle”. It was noted that cold streams within DM halos are supported by the DM filaments (see, e.g., [46, 85, 181]).

In the interface between the inflow and the disk, if the shock does not form or is sufficiently weak, what additional signatures of recent accretion can be expected? If the inflow possesses a nonnegligible angular momentum, as is expected, it will settle in a plane outside the growing stellar disk, but the orientation of this plane can differ significantly from the stellar disk plane, ultimately forming either inclined or polar stellar rings, stellar warps, etc. [185]. It was also shown that mutual orientation of the disk rotation axis, DM halo, and accreting gas fluctuate dramatically over time, even during quiescent periods of evolution, i.e., between major mergers [156]. Misalignment between the halo equatorial plane and the stellar/gaseous disk can be long-lived [43].

Cold flows in the phase space: The maximum information about kinematics of filamentary cold flows is provided by the phase space. It is especially suitable in order to trace the phase mixing, violent relaxation and other associated processes. Comparison of the evolution of pure DM and DM+baryon models in various 2D planes reveals the effect of the baryon inflow on the kinematics of the DM halo [156]. (See Video 5, page xiii.) Both major and minor mergers as well as substructure can be easily distinguished and appear much more prominent before their tidal disruption, by a factor of ~ 2 , in the baryon presence. Moreover, smooth accretion can be well separated from substructure. The tidal disruption itself produces “fingers” which appear more pointed and noticeable in the presence of baryons. The resulting “shell” structure reveals inefficient mixing of merger remnants in the form of velocity–radius correlation. The resulting “streamers” are observed to be long-lived. After $z \sim 1$, the forming streamers survive largely due to $z = 0$. The phase space also delineates the kinematic differences of the inner DM halos which are determined by the gravitational potential shape differences. In summary, the phase-space analysis supports the view that DM halos after reaching virial equilibrium are far from being relaxed in other aspects.

7.7. Conclusions

Galaxies form, evolve and perish — a process that is currently on the forefront of astronomical research. Secular evolution of galaxies is an ongoing process and individual objects participate in this since their formation at some redshift, down to its destruction or to $z = 0$, which can be comparable, in some cases, to the Hubble time. While galaxies of course are born and evolve in conjunction with their environment, as they grow, internal processes are triggered and begin to compete with the external factors. This competition is making the understanding of the galaxy evolution such a complex problem. Of course, one can take a simplifying approach by assuming that galaxy evolution is driven by external processes only, and neglect the internal processes, and vice versa. However, this approach is destined

to fail, as it neglects the intricate mechanism by which the nature operates over time and space. On the other hand, in order to understand the essential physics for this evolution, it is imperative first to simplify the system by neglecting the external factors and focusing on isolated objects, their internal dynamics, and associated processes, like star formation, feedback, chemical evolution, etc. Bringing upfront the full “kitchen” will not help to resolve the main problem, rather it makes the problem intractable.

The last few decades have contributed immensely to our understanding of galaxy evolution, thanks first to development of extraordinary observational facilities at all wavelengths, both ground- and space-based. Secondly, the appearance of the virtual experiment in astronomy — numerical simulations, put our search for structure formation in the universe on equal footing with the rest of physics, which is an experimental science after all.

In this relatively short essay on secular evolution of galaxies, we have attempted to survey some basic and relevant processes which have been analyzed by means of powerful numerical simulations. While there have been clear successes on this road, they have triggered more questions. On top of this, a number of fundamental issues remain unanswered, such as the origin of galactic bars — an issue of such importance that it was and remains the cornerstone of the Hubble Fork diagram. If one of the prime goals of our research is understanding the formation of the Hubble Fork, we are still at the beginning of the process. Approaching the Hubble diagram from another end, we still are sufficiently unsure about the origin of spheroids, i.e., the early type galaxies.

However, over the last couple of decades, we have advanced substantially in our explanation for the large-scale structure in the universe. Under investigation now is structure formation on galactic and subgalactic scales.

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Chapter 8

Cosmic Gas and the Intergalactic Medium

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Diffuse gas outside of galaxies plays an enormously important role in the evolution of the universe. In this chapter, we describe the physical processes and numerical models of cosmic gas from the CMB to the present day. We begin by outlining the basic theory for the thermal evolution of the gas, before taking an approximately chronological ride through a number of important phases: the evolution of gas before reionization, the process of reionization itself, the intergalactic medium and the Lyman- α forest, and finally ending with a discussion of the circumgalactic medium. We highlight both the key numerical results and outstanding questions throughout.

8.1. Evolution of diffuse gas in the Universe

In this chapter, we will focus on the physical processes, numerical simulations, and observational probes of diffuse “cosmic” gas. Although diffuse gas can certainly exist within galaxies (indeed, much of the volume of the Milky Way’s ISM is composed of low-density gas), we will largely stay out of galaxies in this chapter, choosing here to focus on low-density gas which is not *directly* affected by star formation or AGN. This will help to simplify the physics, and indeed a general understanding of how diffuse gas evolves is relatively straightforward, and is generally easy to capture in numerical models. This is particularly true at early times, before galactic winds have polluted much of the universe, and many (but not all) of the simulations and observational probes that we discuss are relatively robust to the uncertainties involved in modeling feedback from stars and AGN. On the other hand, we are well out of the linear evolution of the early universe and the

Cosmic Microwave Background, and numerical models are required to understand the evolution of the gas, and (eventually) calibrate simpler analytic or semianalytic models.

The review is organized around four (somewhat overlapping) epochs in the history of diffuse gas. In each case, we will begin by describing the key physical effects and how they are modeled before going on to discuss the existing observations and numerical simulations that have been used to model them. We will begin in the cosmic dark ages (completely skipping the production of the cosmic microwave background), when the universe was primarily neutral, before exploring the process of hydrogen reionization, and then moving on to the evolution of the intergalactic medium (IGM), which lies outside of the virial radius of collapse halos, and the circumgalactic medium (CGM), which lies within. We highlight a few open questions throughout. This review is not primarily historical, but will note a number of seminal works along the way. Other recent reviews include [1–3].

8.1.1. *The thermal evolution of diffuse gas*

The essential fluid equations and the numerical methods for solving them are discussed in Chapter 3 and we will not repeat them here, instead focusing on the thermal evolution of the gas. We will lay out the equations in this section, and discuss solutions for specific regions (reionization, IGM, etc.) in more detail in the sections below. The temperature of a Lagrangian fluid element with temperature T evolves as

$$\frac{dT}{dt} = -2HT + \frac{2T}{3\Delta} \frac{d\Delta}{dt} - \frac{T}{n} \frac{dn}{dt} + \frac{2}{3k_B n} \frac{dQ}{dt}, \quad (8.1)$$

where $H(z) = \dot{a}/a$ is the Hubble constant, Δ is the baryonic density of the fluid element in units of the mean baryonic density n . The first two terms on the right simply encode the conservation of entropy, with the first term arising from the homogeneous cosmological expansion and the second term coming from evolution of the (Lagrangian) fluid element, relative to the mean. This split is somewhat artificial since conservation of entropy implies $K = T/\rho^{2/3}$ is constant for an adiabatic process, but is typical of how many numerical simulations are actually implemented (i.e., in comoving coordinates) and allows us to immediately see that gas with constant overdensity evolves as $T \propto (1+z)^{-2}$. The third term just reflects the change in temperature due to the changes in the number of particles at fixed mass density and is important mostly during reionization. The last term describes the effects of both radiative cooling and heating. This entire equation is only valid outside of shocks, within which the entropy (and temperature) rises. We refer readers in search of more details to Refs. [4–7].

The radiative heating and cooling may include a wide variety of processes; however, before metal enrichment, the relevant number of processes is relatively

limited:

$$\frac{dQ}{dt} = \Gamma_{\text{Compton}} - \sum_i \Lambda_i(T) n_e n_i + \sum_i \Gamma_{\text{photo},i} n_i. \quad (8.2)$$

The first term describes Compton cooling or heating (almost always due to the CMB for diffuse cosmic gas), the second term describes cooling due to recombination, excitation and possibly bremsstrahlung of species i (where we will consider mostly low metallicity gas and so assume that i is one of H, He, and He^+), while the final expression represents photoionization heating of species i , which depends on the strength of the (angle-averaged) specific intensity J_ν above the ionizing threshold of that species (ν_i):

$$\Gamma_{\text{photo},i} = \int_{\nu_i}^{\infty} \frac{4\pi J_\nu \sigma_i(\nu) (h\nu - h\nu_i)}{h\nu} d\nu, \quad (8.3)$$

where $\sigma_i(\nu)$ is the ionizing cross-section of species i .

The temperature evolution is generally reasonably simple and is set by usually only one or two rates at a time, as we will discuss in more detail in the sections below. Note that the left-hand side and first two terms of Eq. (8.1) can be written even more simply as $n^{2/3} dK/dt = 0$ in terms of the conservation of an entropy-like quantity $K = T/n^{2/3}$. This makes it clearer that we are assuming constant entropy (in the absence of radiative cooling or heating). When a fluid element accretes onto a dark matter halo, it usually will experience an accretion shock, boosting the entropy by $\Delta K_{\text{acc}} \approx (v_{\text{acc}}^2/3)(\pi r_{\text{acc}}^2 v_{\text{acc}}/\dot{M}_{\text{acc}})^{-2/3}$, where v_{acc} , r_{acc} , and $\dot{M}_{\text{acc}}$ are the accretion velocity, radius, and mass inflow rate, respectively (these can often be taken to be the quantities close to the virial radius).

The number density of each species depends on the recombination and ionization rates. To determine these, we solve a kinetic network for the rate of change of species density n_i with the general form

$$\frac{\partial n_i}{\partial t} = \sum_j \sum_l k_{jl} n_j n_l + \sum_j I_j n_j, \quad (8.4)$$

where k_{jl} is the rate for reactions involving species j and l while I_j is the appropriate radiative rate. Note that in rare cases there may be an additional term for three-body reactions. In this review, we will be primarily interested in the abundance of one species: H, which is governed by:

$$\frac{\partial n_{\text{HII}}}{\partial t} = \Gamma_{\text{HI}} n_{\text{HI}} - \alpha(T) n_{\text{HII}} n_e, \quad (8.5)$$

where $\alpha(T)$ is the recombination rate and Γ_{HI} is the ionization rate for hydrogen:

$$\Gamma_{\text{HI}} = \int_{\nu_i}^{\infty} \frac{4\pi J_\nu \sigma_{\text{HI}}(\nu)}{h\nu} d\nu. \quad (8.6)$$

Finally, we have ignored the (nonradiative) input from stars. The primary impacts are the addition of metals and energy from galactic winds — we will defer a discussion of enrichment until the last two sections; fortunately, they have only a minor impact on gas in the IGM.

8.2. Cosmic gas in the dark ages

After recombination at $z \approx 1200$, the IGM is largely neutral, with a residual ionization fraction of $\sim 3 \times 10^{-4}$. Although low, this is still sufficiently high for Compton heating from CMB photons to maintain the gas temperature close to the CMB temperature until $z_{\text{dec}} \approx 150(\Omega_b h^2 / 0.023)^{2/5}$ [8]. At that point, it thermally decouples, reaching a temperature of ~ 180 K at $z \sim 100$, beyond which the temperature drops at $(1+z)^2$ for gas at the mean density. Detailed calculations can be computed with the numerical tool RECFAST [9], which includes a large number of radiative processes, but only holds in the homogeneous limit.

Once structure begins to form, along with the first stars and quasars (see Chapter 4), the radiative background begins to build up. Due to the high densities at early times, photoionizing UV radiation has a very short mean-free length and most diffuse gas sees only low-energy photons (below the HI ionizing edge at 13.6 eV), or high-energy photons, such as X-rays. The low-energy photons generally do not interact with the mostly neutral gas, while hard X-rays have a long path length and heat the gas largely through secondary ionizations. The primary source of X-rays is likely high and low mass X-ray binaries (HMXB, LMXB), although the formation of such systems at high redshift is quite uncertain. This means that the resulting temperature of the IGM is also uncertain — a recent example of the heating rates and resulting temperature evolution is shown in Fig. 8.1, (from [10]). As the plot shows, at early times, HMXBs, which form promptly, likely dominate the X-ray

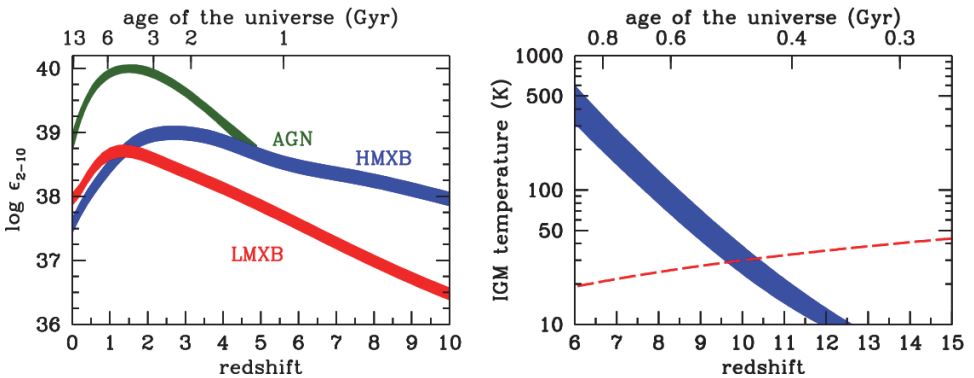


Fig. 8.1. The left panel shows an estimate of the 2–10 keV X-ray emissivity from three classes of sources (as labeled), while the right-hand panel shows the resulting temperature of the IGM (blue curve). The red dashed curve shows the CMB temperature. Both panels are taken from [10].

production, while later on Active Galactic Nuclei (AGN) are the leading source below $z \sim 4$ (although this occurs after reionization and so gas heating is dominated by photoionization). These sources heat the gas from the very low temperatures that result from adiabatic expansion, rising above the CMB temperature at $z \sim 10$ (although, again, exact numbers are quite uncertain and depend sensitively on the X-ray production efficiency at high redshift).

8.2.1. 21-cm tomography

One way to probe fluctuations in this early pre-reionization period, during which the hydrogen is largely neutral, is through fluctuations in the redshifted 21 cm fine structure line [11–13]. This line is very challenging to observe, since it is very faint compared to known foregrounds, however, its spectral properties compared to the foregrounds should allow its detection. The offset of the 21-cm brightness temperature from the CMB temperature is given by

$$\delta T_b(\nu) = \frac{T_s - T_{\text{CMB}}}{1 + z} (1 - e^{-\tau_{\nu_0}}), \quad (8.7)$$

where T_s is the gas spin temperature and τ_{ν_0} is the optical depth at the 21-cm frequency ν_0 (which is redshifted to different frequencies by cosmological expansion, allowing us to probe the three-dimensional structure of the gas). At early times, the spin temperature may be below the CMB temperature, and the 21-cm line may be in absorption (although this depends sensitively on coupling between the 21 cm spin temperature and the gas temperature, which is set by both collisions and photon interactions — see [14] for a discussion of this coupling). However, this period will be challenging to observe, and most 21-cm tomography investigations focus on the more observable period around reionization where $T_s \gg T_{\text{CMB}}$.

8.3. Reionization

Reionization is a particularly challenging period to model as it effectively couples both large and small scales. In addition to modeling the dark matter and gas dynamics, as described in Chapters 2 and 3, and the thermal and chemical evolution as described earlier in this chapter, we must also follow the inhomogeneous distribution of ionizing radiation. This final aspect means solving the equation of radiative transfer as well as developing a prescription for the sources of that radiation (stars and quasars).

8.3.1. Numerical radiative transfer

In this section, we briefly summarize a variety of approaches to numerical cosmological radiative transfer; see, for example, [3] for a more complete review. The specific intensity I_ν with frequency ν along a direction $\mathbf{n}$ evolves in an FRW universe

according to the following equation:

$$\frac{\partial I_\nu}{\partial t} + \frac{c}{a} \mathbf{n} \cdot \nabla I_\nu - H \left(\nu \frac{\partial I_\nu}{\partial \nu} - 3I_\nu \right) = -k_\nu I_\nu + S_\nu, \quad (8.8)$$

where k_ν is absorption coefficient (which depends on gas properties) and S_ν is the source function, which encodes the production rate of radiation (and so requires knowledge of the star/quasar distribution). Because of the six-dimensional nature of this equation (three spatial dimensions, two angles and frequency), it is computationally demanding to solve. In addition, simple analytic models are of less use in cosmology, where generally sources do not fill their Stromgren spheres, and are constantly evolving due to the changing density caused by cosmological expansion and structure evolution. There are three main ways to solve these equations in the cosmological context: moment-based methods, Monte Carlo techniques, and ray tracing.

In the first, moments of the radiative transfer equations are taken by multiplying Eq. (8.8) by powers of the photon angles and integrating over all angles, in a manner very analogous to that used to compute the fluid equations from the Boltzmann equation. Usually, the quantities actually evolved are the radiation energy density and the (vector) radiative flux, i.e., the first and second moments (either integrated over all frequencies, or perhaps a range of frequencies). The evolution equation for the energy density depends on the flux, and the evolution equation for the flux depends on the third moment, a quantity typically called the Eddington tensor, so in order to close the hierarchy, an approximate and fast way of computing this tensor (which is usually normalized by the radiation energy density to make it dimensionless) must be found. Examples of this technique include: Gnedin and Abel [15] and Petkova and Springel [16], who developed an optically thin approach; Aubert and Teyssier [17], who used a local (“M1”) closure, and Finlator, Özel, and Davé [18], who used long characteristics. The even simpler flux-limited diffusion approach, where the Eddington tensor is a simple function of the local energy density, has also been used in cosmological models [19, 20]. Typically, these methods scale as $\mathcal{O}(N_{\text{RT}} \log N_{\text{RT}})$, where N_{RT} is the number of radiative elements; this scaling is typically quite fast, although the accuracy of these approaches depends sensitively on the closure adopted and the radiative field to be modeled.

Monte Carlo methods sample the radiation field using a ray-casting method to evolve discrete photon packages that have random directions (and possibly frequencies). The photon packets are produced by a set of sources and are then evolved directly with the radiative transfer equations. Due to the random sampling, such methods can be noisy and convergence may be slow; however, relatively few approximations are required. The scaling is generally $\mathcal{O}(N_s N_p)$, where N_s is the number of sources and N_p the number of photon packets emitted by each source. Examples of this technique include Refs. [21–24].

Finally, the most popular category is the ray-tracing techniques. This includes short characteristic methods (e.g., [25–29]) in which the equation of radiative transfer is integrated only along a relatively small number of directions to nearby cells. The advantage of this method is that it has excellent scaling properties — linearly as $\mathcal{O}(N_{\text{RT}})$ — and it can be easily parallelized. The disadvantage is that it is relatively diffusive in direction, which can be particularly problematic in cases in which a small number of sources dominate the radiative input to a large region.

To get around this problem, long characteristic methods solve the radiative transfer equations along rays which go from each source to each affected cell or particle. In the most straightforward implementation, each source emits a fixed number of rays with an isotropic distribution such that each ray contains the same number of photons. To properly account for multiple sources interacting, rays are cast cell-by-cell, with a timestep given by $\Delta t \sim \Delta x/c$, where Δx is the resolution element size and c the speed of light. To get around this short timescale, simulations often employ a reduced speed of light approximation [15, 30]. The scaling of this simple scheme is $\mathcal{O}(N_s N_{\text{RT}})$, which in the case of many sources can be as bad as $\mathcal{O}(N_{\text{RT}}^2)$. The large number of rays is required by the possibility that a source may reach over the entire grid before all of its photons are absorbed; however, when the path length of typical sources is much smaller, significant improvements can be made by introducing an adaptive ray-tracing method [31]. Further improvements can be made by merging nearly parallel rays from different sources [32, 33].

One challenge with all of these methods is determining the accuracy and robustness of the results. To help answer these questions, a pair of papers [34, 35] has suggested and carried out a systematic set of radiative transfer tests, ranging from idealized cases to cosmological density distributions.

8.3.2. *Results of reionization simulations*

These numerical methods have been used to study the process of cosmological reionization, although progress is challenging for two reasons. First, the formation of stars and the escape of radiation from high redshift galaxies is poorly understood, so the source function in the radiative transfer equation is usually taken to be proportional to the star formation rate (and possible black hole accretion rate) with a coefficient set to match observations. Second, simulations must cover a very large range of scales, from the smallest halos, which can produce stars (approximately $10^8 M_\odot$), to the scale of ionizing bubble overlap, which can be large (~ 100 Mpc) due to the clustering of sources [2]. Although we are not yet able to model this large range, simulations are getting close and the basic features of reionization are becoming clearer.

The source of the ionizing photons at high redshift is almost surely dominated by stars in galaxies, as the observed quasar population is insufficient [37]. However, as noted above, even the highest resolution cosmological simulations do not resolve the detailed gas dynamics in galaxies and so cannot predict their escape fractions,

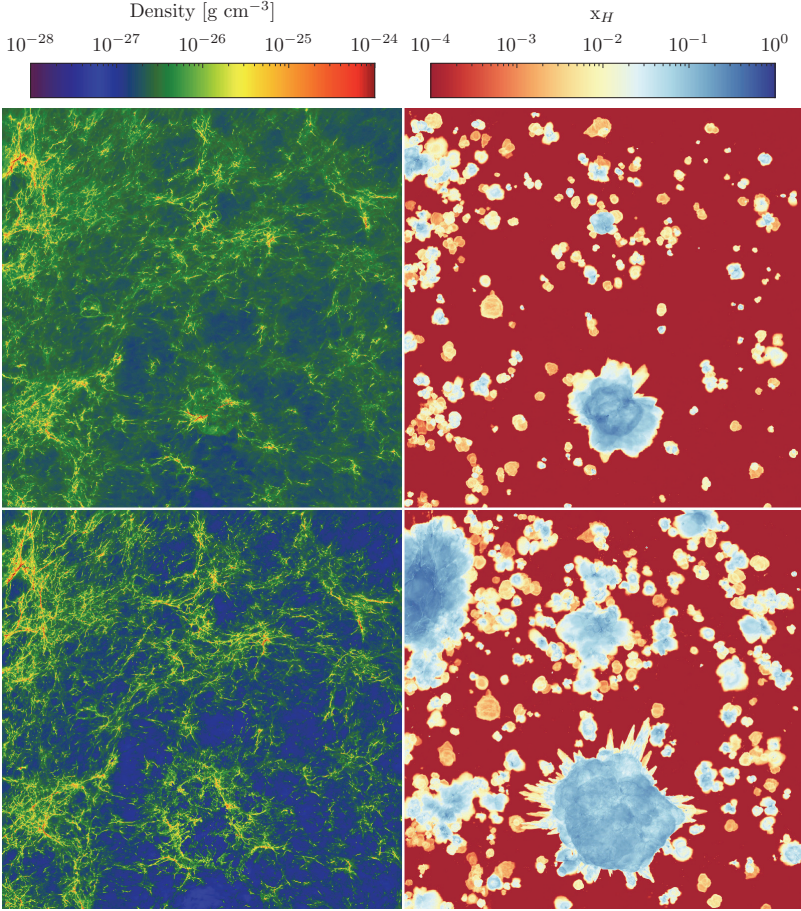


Fig. 8.2. Projections of density-weighted baryon density (left) and hydrogen ionization fraction (right) at $z = 15$ (top) and $z = 12.5$ (bottom). (Figure taken from [36].) The projected volume is a cube with side of 6.1 comoving Mpc.

although focused and idealized simulations have begun to make progress in this area [38, 39]. In Fig. 8.2, we show an example of such a high-resolution model, which includes a model for both Pop III and Pop II star formation at a resolution sufficient to model both the radiative and energetic feedback from stars, although this is too computationally costly to model a large enough region for long enough to see the process of reionization complete.

Generally, such simulations have found that while very low-mass systems allow a majority of their ionizing photons to escape, more massive systems ($M > 10^9 M_\odot$) have lower escape fractions, although they can still dominate the ionizing radiation production due to their higher star formation rate. For example, Fig. 8.3 shows the mean escape fraction and ionizing photon production from the same set of

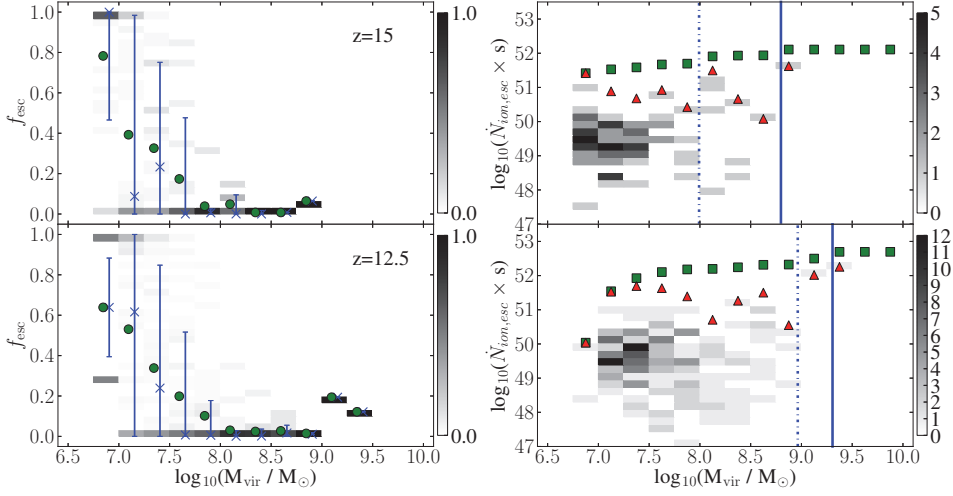


Fig. 8.3. Distribution of UV escape fraction (left) and number of escaped photons (right) as a function halo virial mass at $z = 15$ (top) and $z = 12.5$ (bottom). The mean escape fractions in 0.25 dex bins are represented by green filled circles. The median escape fractions are represented by blue crosses, and 15 and 84 percentiles are shown as the bottom and top of vertical lines. The number of escaped UV photons from galaxies and the cumulative number of escaped UV photons are represented by red triangles and green squares, respectively. Figure taken from [36].

simulations as in Fig. 8.2. They found that this was driven in part by short bursts of star formation during which the escape fraction increased above quiescent periods.

This picture may be consistent with observations of high-redshift galaxies, an area in which significant progress has been made in the past few years. For example, recent observations [41] have probed down to star formation rates of $0.1 M_{\odot}/\text{yr}$ at $z \sim 9$, finding that, even down to these low limits, the observed systems are unable to produce enough ionizing photons given typical (low) estimates for their escape fractions. However, as expected from simulations, the lower mass galaxies may be able to make up for this deficit and simulations of the entire process, given reasonable ionizing photon production rates and escape fractions can now match a wide range of reionization observables. For example, the recent Aurora suite of simulations [40] uses an SPH-based radiative transfer solver in a box which is large enough to resolve much of the clustering to reproduce observations of the evolution of the hydrogen neutral fraction and Planck observations of the electron scattering optical depth encountered by CMB photons (recently revised to lower values). These results are shown in Fig. 8.4.

Even larger numerical simulations are able to resolve the topology of reionization (although at the cost of poorer resolution at the low mass end of galaxy formation). Early in the study of reionization, there was much analytic discussion of whether the process would be inside-out, in which the densest peaks were ionized first (due to sources embedded inside of them) or outside-in, in which ionizing

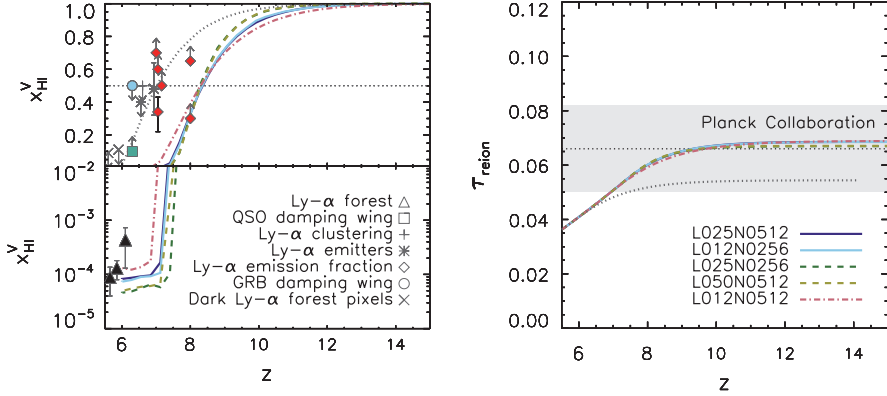


Fig. 8.4. The left panel shows reionization histories from the Aurora suite of reionization simulations, compared against a range of observation probes (see [40] for details). The right panel shows the predicted optical depth for CMB photons with the observed range from Planck shown in gray. Figure taken from [40].

photons escaped from the first halos and quickly ionized the low-density void regions, only slowly ionizing the denser peaks. In fact, neither picture is fully correct, and simulations [42] have generally shown that the process progresses in multiple phases, with the first primarily inside-out, with the first generation of sources ionizing bubbles around them, followed by a rapid overlap in which the ionized volume fraction climbs quickly to one and the mean ionizing background grows quickly, followed by a more gradual ionization of the remaining dense filaments.

This picture supports the use of analytic or semianalytic models [43] which use the excursion-set approach (the basis of analytic method of computing the halo mass function) to create simple and fast models of reionization based on the idea that star formation, and hence the production of ionizing photons, occurs in denser regions smoothed on a specific scale, and then propagates outward. This approach can be used to make fast estimates of the predicted 21 cm signal [44] and other observables. During reionization, the HII regions appear as holes in the observed 21 cm signal and should tell us much about the topology of reionization.

8.4. Intergalactic medium

In the immediate aftermath of reionization, the mean free path of ionizing photons is short, resulting in significant fluctuations in the intensity of the radiation field: to a good approximation the local radiation field is determined by the sources within one mean free path and when this is short, the number of sources inside of that volume is small, resulting in significant variations in the radiation field. At this stage, radiative transfer calculations are still required. As time goes on, the mean free path of ionizing photons grows, and the fluctuations in the ionizing background drop, allowing us to simplify the evolution by assuming that the background is constant

except for the effect of local self-shielding. However, even that is unimportant in the diffuse intergalactic medium (IGM), and for $z \lesssim 5$, we can assume that the gas is optically thin (except in the vicinity of QSOs, where the ionizing radiative strength may be significantly boosted). This greatly simplifies models of the IGM, which is very useful since the Lyman- α forest is a key observable for such gas, as we will discuss in more detail in the next few sections. In this regime, the gas quickly reaches ionization equilibrium and, for the low densities of the diffuse IGM, is well approximated by,

$$n_{\text{HI}} = \Gamma_{\text{HI}} \alpha(T) n^2 \propto \Gamma_{\text{HI}} T^{0.7} \Omega_b^2 \Delta^2, \quad (8.9)$$

where $\alpha(T)$ is the HI recombination rate and the second proportionality uses the temperature dependence of the recombination coefficient ($\alpha \propto T^{0.7}$). This means that if we know the temperature, the hydrogen number density (directly observable through the Lyman- α forest) can be used to determine the baryon density, and hence important cosmological information.

8.4.1. *Temperature evolution: Theory*

The gas temperature is not quite as simple, but the broad outlines are well understood [4]. First, reionization of a given fluid element occurs rapidly and boosts the temperature to approximately $1\text{--}3 \times 10^4$ K. The precise temperature depends on the spectral shape seen by the gas element, which is a challenging problem in detail [45]. In principle, stellar sources are soft and most early simulations assumed the optically thin limit during reionization. Since gas heating comes from the excess energy of photons above the ionization edge at $h\nu_0$ (i.e., each photon brings an energy of $h\nu - h\nu_0$), a soft spectrum means a low gas temperature. However, by the time an ionization front reaches a typical fluid element, many of the softer photons (which have shorter mean free paths) will have been absorbed, meaning that the typical temperature of the gas is hotter than might be expected [45], although there is an effective upper limit to the temperature (around 3×10^4 K) due to rapidly increasing energy losses (at these temperatures, the neutral atoms are easily excited and rapidly decay). Note that fluctuations in the gas temperature can arise both due to changes in the spectrum of the ionization radiation (due to radiative transfer effects) and to the fact that reionization occurs at different times in different places.

After being heated during reionization, the gas temperature evolves more slowly, responding to adiabatic cooling, and (primarily) photoheating of ionized gas that recombines. As shown by analytic work and full numerical simulations [4], the gas rapidly moves towards a tight relation between baryonic density and temperature. This occurs because the photoheating rate (which dominates the heating, and is, in turn, controlled by the recombination rate) is nearly proportional to $n_H^{2/3}$, resulting in $dK/dt = \text{const}$, causing the gas to continually gain entropy at a constant rate, eventually erasing memory of its initial state. The asymptotic relation considering only photoheating and adiabatic expansion is found to be $T \propto \Delta^{3/5}$ (close to the

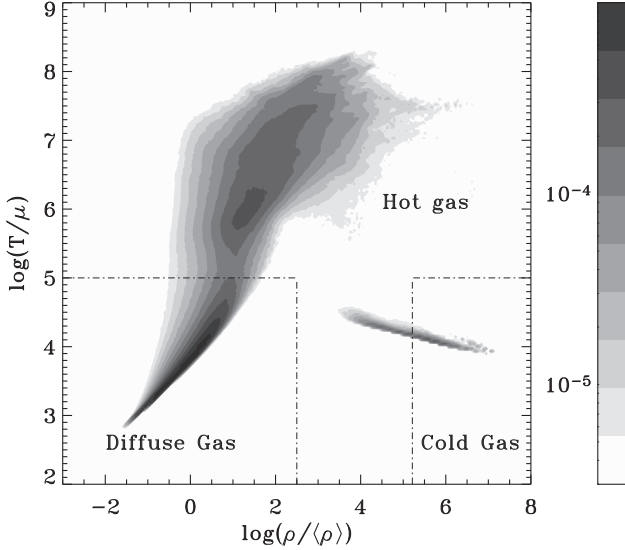


Fig. 8.5. Phase diagram of the baryonic gas from a full cosmological simulation at $z = 0$. Grayscale shows the mass-weighted distribution of gas at each density and temperature with labels for cold diffuse gas, hot (shocked) gas, and cold gas in galaxies. Figure taken from [46].

isentropic $2/3$ relation). Other processes, such as Compton cooling and recombination cooling are of lesser importance (particularly for high reionization temperatures) but tend to accelerate the convergence toward a simple power-law relation between the gas temperature and density [6].

Based on this analytic and numerical work, the temperature–density relation of the diffuse gas is often approximated with a power-law:

$$T = T_0 \Delta^\alpha, \quad (8.10)$$

where α is typically between 0.3 and its asymptotic value of 0.6.

In Fig. 8.5, we show the distribution of baryonic density and temperature from a numerical simulation. The tight density–temperature relation of the IGM can be easily seen (marked “Diffuse gas”), even at $z = 0$. At higher redshifts, even more of the universe’s baryons are in this phase (in fact, by $z \sim 3 - 4$, this phase dominates the baryon census of the universe). The hotter gas represents shocked baryons, generally in the CGM of halos, which we will discuss more in following sections, and the cold, dense gas in the lower-right corner of the diagram is found mostly in galaxies.

8.4.2. *Lyman- α forest*

The single best probe of the IGM comes from HI absorption lines in distant quasars. This works because photons emitted by the quasar along the line of sight to us are

scattered by the remaining neutral hydrogen atoms when their redshifted wavelength matches a resonance transition, the most important of which is the H $n = 2$ to 1 line (the Lyman- α line) at $\lambda_0 = 1216 \text{ \AA}$, although other transitions in hydrogen (in particular, the Ly- β forest), helium, and heavier elements can also be significant. The underlying emission of the quasar is smooth (since lines are usually very broad) and is typically modeled with a smoothly varying function $F(\lambda)$, which is then decreased by scattering from the Lyman- α forest, so that the observed flux is $F(\lambda)e^{-\tau}$, where the optical depth τ for the Lyman- α transition, and hence the depth of the absorption line, is given approximately by

$$\tau(\lambda) \propto \frac{\Omega_b^2 H_0^2 (1+z)^3}{\Gamma H(z)} \alpha(T) \Delta^2, \quad (8.11)$$

where Δ and T are the overdensity and temperature of the gas that is redshifted such that it absorbs at $\lambda = \lambda_0(1+z)$. So we see that the absorption is a direct probe of the IGM density and temperature (although note that this expression is modified by peculiar velocities of the gas [48]). In fact, given the density-temperature relation described earlier, Eq. (8.10), the optical depth depends only on the baryonic density as Δ^β with $\beta \approx 2 - 0.7\alpha$.

An example Lyman- α spectrum of a quasar is shown in Fig. 8.6, which demonstrates its remarkable ability to trace the low density IGM. Due to the combination

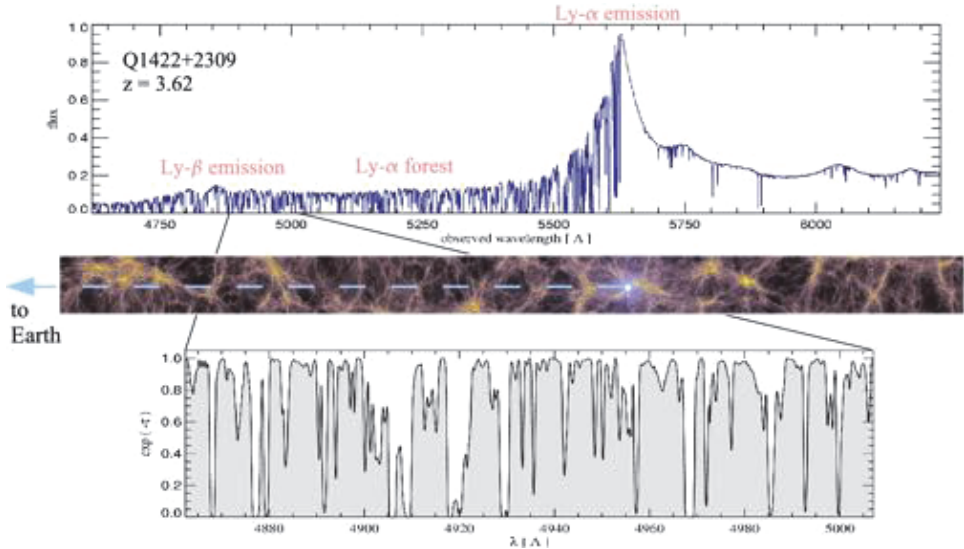


Fig. 8.6. The top panel shows a typical spectrum of a quasar at redshift $z = 3.62$ with the Lyman- α and Lyman- β emission lines of hydrogen labeled. These come from the quasar, but the forest of absorption lines shortward of the Lyman- α peak come from overdensities in the web of diffuse intergalactic gas, an example of which is shown in the middle panel. The bottom panel shows a blow-up of a portion of the quasar spectrum, now normalized by an estimate of the quasar spectrum to show the detail in the absorption lines. Figure taken from [47].

of the large cross-section of neutral hydrogen and the brightness and spectral smoothness of quasars, we can probe baryon fluctuations which have overdensities as low as $\Delta \sim 1$ and comoving wavelengths approaching an Mpc. This is in contrast to most galactic observables which give us information primarily about the highly nonlinear regime or a biased view of longer wavelengths.

Early analysis of the Lyman- α forest focused on fitting individual absorption lines with Voigt profiles [51], which worked well for simple systems and even today allows for a more direct connection between the absorbing gas and the physical quantities (such as column density) and is still used for Lyman-limit and damped Ly α systems, which arise from denser gas and are generally associated with galaxies or their immediate halos.

In Fig. 8.7, we show the result of comparing real and mock spectra, analyzed in this way, by looking at the distribution of absorbers, ranging from column densities of $10^{12.5} \text{ cm}^{-2}$, which are at the limit of the noise even in these high-resolution, high signal-to-noise spectra, up to the Lyman-limit edge. This figure demonstrates both the large number of low column-density absorbers as well as the remarkable success that modern cosmological hydrodynamic simulations have in reproducing the

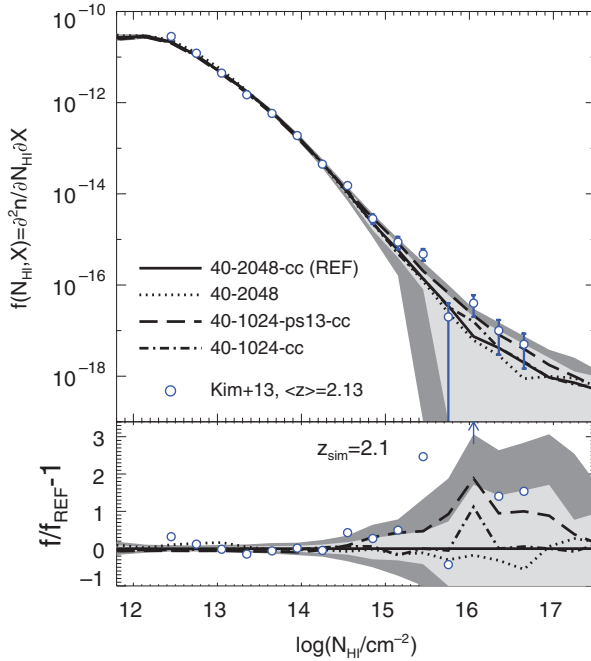


Fig. 8.7. The distribution of Lyman- α forest lines as a function of column density, at $z = 2.1$. The open circles show observed data from 18 high-resolution quasars; from [49], while the solid and dashed lines show a variety of numerical simulations, with different resolutions and feedback models, demonstrating the robustness of this prediction. The bottom panel shows the fractional deviation from the reference simulation. Figure taken from [50].

observed distribution of absorbers. Because these systems are usually low-density filaments and walls in the cosmic web and are far from galaxies, the impact of uncertainties in numerical simulations, as well as subgrid models such as star formation and feedback prescriptions are minor, only impacting the high-column densities absorbers, which tend to be clustered near to galaxies (or even in their CGM — see Section 8.6). This means that the only uncertain astrophysical parameter (i.e., aside from cosmological ones) is the intensity of the ionizing background. The impressive agreement in such figures can be seen as a strong check on our underlying cosmological model.

However, fitting spectra with Voigt profiles can produce ambiguous results when multiple profiles are required to fit a feature or set of features, and at higher redshift the density of absorbers becomes very high, making the fitting procedure degenerate. Therefore, often the analysis is based on other ways to characterize the flux distribution, such as computing the power spectrum of the Fourier transform of $\delta_F = F/\langle F \rangle - 1$, where the flux has been normalized (and possibly had its distribution function changed into a Gaussian). Alternate approaches are to compute the covariance matrix of δ_F directly in real space, which can then be Fourier transformed to get the power spectrum. For a recent example of this approach, in Fig. 8.8, we show the one-dimensional flux power spectrum measured from 14,000 quasar spectra from the Baryon Oscillation Spectroscopic Survey (BOSS) [52].

The power spectrum determined in this way can be compared to numerical simulations of the IGM. Although the fluctuations are not in the linear regime, as for the CMB, the calculation is actually quite robust for a number of reasons: (i) the exponential dependence of the flux on the optical depth (and hence Δ)

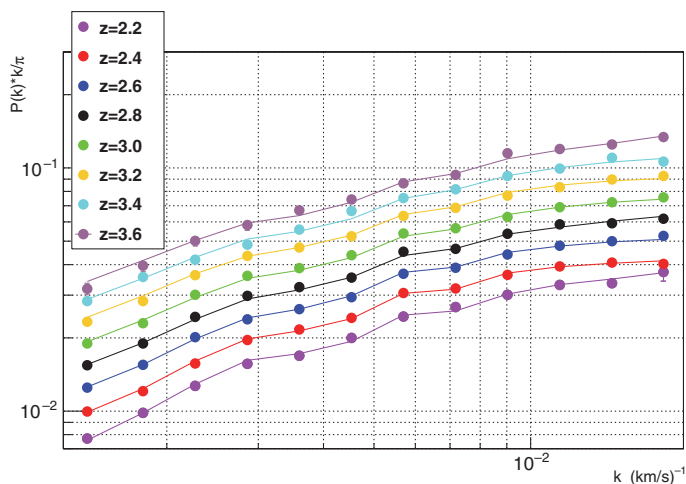


Fig. 8.8. The measured power spectrum (along with an empirical fit) of the power spectrum measured from 14000 quasar spectra from the BOSS survey in the range $z = 2-4$. Figure taken from [52].

means that we are not sensitive to very large overdensities — most of the signal comes from moderate values of Δ ; (ii) the relation between the overdensity (Δ) and the observable (F) involves relatively well-understood physics and can, in principle, be exactly computed.¹ This can be contrasted to galaxy number counts where the relation between the observed and predicted overdensities depends on a bias parameter, which must be observationally constrained. Due to the mildly nonlinear nature of the Lyman- α forest, relatively low-resolution hydrodynamic simulations are perfectly adequate and it is generally thought to be insensitive to the uncertain physics of galaxy and quasar feedback.

In addition to looking at the correlation between pixels within a single spectrum, surveys which observe many quasars densely on the sky can measure the correlation of pixels between closely separated quasars, as done by the SDSS [54]. This provides even tighter cosmological constraints and allows the measurement of various cosmological features; for example, by comparing the correlation function parallel and perpendicular to the line of sight, the Alcock–Pazynski test can be used to constrain redshift-space distortions, and, on longer scales, the Baryonic Acoustic Oscillations (BAO) can be measured [52].

The results of these observations and simulations produce very tight measurements on the cosmological power spectrum on length scales smaller than almost any other probe (down to wavelengths of a comoving Mpc, or even lower, at redshifts $z \sim 3$) and represent some of our best constraints on the presence of massive neutrinos [55], and warm dark matter candidates. Figure 1.4 in Chapter 1 shows the power spectrum of density fluctuations from the Lyman- α forest compared to other sources, from the CMB to weak lensing, demonstrating the unique small-scale role played by this probe of diffuse gas.

8.5. Temperature evolution of the IGM: Observations

The Lyman- α forest can also be used to measure the temperature of the IGM, allowing us to test the theoretical description of the thermal history outlined in Section 8.4.1. This can be done in a variety of ways — for example, the width of individual Voigt profiles depends on the temperature of the gas in a predictable fashion (although also on the velocity structure of the gas) [56]. Other methods include Fourier transforming the spectrum, or fitting it with wavelets or similar filters, and looking for the sharpness of such features. These are all based on the idea that increased temperatures would effectively smooth the spectrum — indeed, one alternative method is to measure the distribution of second-derivatives (“curvature”) of the flux spectrum to directly probe the sharpness of the spectrum [57].

In Fig. 8.9, we show a compilation of observations of the IGM temperature using a variety of methods at redshifts from $z = 2$ to 6. As discussed

¹Although one of the biggest remaining stumbling blocks to higher precision constraints remains the uncertain thermal evolution of the IGM.

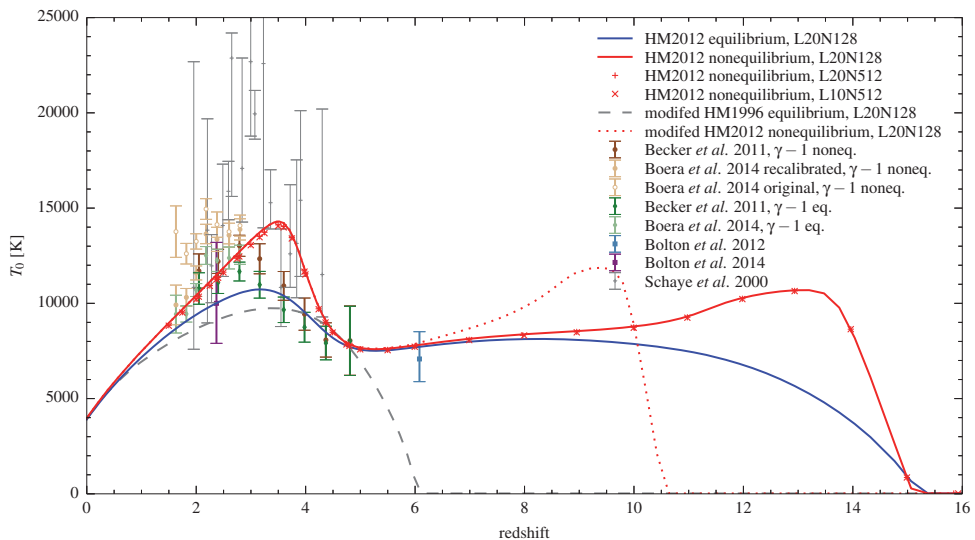


Fig. 8.9. The evolution of the IGM temperature at the mean density (i.e., at $\Delta = 1$). Lines show a range of models as described in the legend, while symbols indicate observed estimates using a wide variety of methods. See [58] for more details on methods and sources. Figure taken from [58].

earlier, the IGM temperature probably depends on density (Eq. (8.10)), and so here we show the temperature at the mean density $\Delta = 1$. The lines in this figure show a variety of models with reionization at redshifts $z = 10$ to 15 . Note that, regardless of the reionization redshift, the temperature at $z \sim 6$ has settled to the same value; this is due to the combination of photoheating and expansion described earlier that drives gas to nearly a constant adiabat. The peak in temperature at $z \sim 3$ is most likely due to the photoionization of HeII driven by the hard spectrum from quasars which dominate at these redshifts. The good agreement between theory and observations seen in this figure is reassuring, however two points are worth making: first, the match is not perfect, and second, there is a lack of comparison data at high-redshift, but even more so at low-redshift.

8.6. Circumgalactic medium

Finally, we turn to cosmic gas close to galaxies. The term circumgalactic medium (CGM) has been coined to denote the multiphase diffuse gas that is within the virial radius of a dark matter halo and not part of the interstellar medium (ISM). In X-ray clusters, this gas is almost entirely hot, but in lower mass halos, may exist in a range of phases from cool to hot. It is challenging to model because it contains a significant amount of the baryons, but spread out over a large region with potentially multiphase gas.

8.6.1. *Gas accretion and the minimum halo mass to host baryons*

We begin by examining the accretion of intergalactic gas onto dark matter halos. For high mass halos, the potential well is deep enough that gas inflow rates closely mirror the dark matter accretion, but in lower mass halos, reionization can heat the gas enough to prevent accretion, resulting in “dark” halos without significant baryonic components. To first order, the mass-scale at which this transition occurs is the Jeans mass evaluated at the mean density for 10^4 K gas. Since the mean density is redshift dependent, it has been suggested that a more accurate value is the average Jeans mass, known as the filtering mass [60].

More recent efforts have established the baryonic evolution in more detail. An example of this is shown in Fig. 8.10, from Ref. [59], demonstrating the evolution of gas clouds collapsing at different redshifts in the density–temperature phase plane. In the top-right panel, we see gas destined for a high-redshift halo collapsing at $z = 6$, corresponding to a turn-around redshift of about $z = 10$, assuming a spherical collapse model. This redshift is very close to the reionization redshift and so the evolution is straightforward: the gas is heated by reionization to $\sim 2 \times 10^4$ K at which point cooling is effective, and the gas accretes onto the halo (assuming the halo mass is above the Jeans mass evaluated approximately at that density and temperature), moving to higher density and lower temperature as it is compressed (here we ignore the effect of the accretion shock, but will return to this point below).

For gas collapsing onto halos at lower redshifts, depicted in the lower two panels of Fig. 8.10, the evolution can be more complicated. Before accretion, it is heated by reionization, and then first expands as it follows the Hubble flow and then contracts after it turns around and starts to recollapse (again, assuming the halo mass is sufficiently large). The temperature evolution during this time is close to adiabatic, although experiencing a net entropy boost due to photoheating, as described in Section 8.4.1. This is seen in the diagram by the dark black lines, which largely follow lines of constant entropy; this continues until radiative cooling becomes important, at which point the temperature follows the blue (equilibrium) curve as it accretes onto the halo.

Although schematically, this picture gives us a better idea of the physical evolution of the gas, and also can be used to improve on the simple filtering mass approximation described earlier. In Fig. 8.10, the green star is the mean (baryonic) density of the universe at each collapse redshift, giving an idea of the difference between the Jeans mass estimated at the mean density and the (smaller) value found for gas participating in the collapse. This method agrees with numerical simulations showing that the minimum halo mass able to host baryons is approximately $10^9 M_\odot$ at $z = 6$, rising to nearly $10^{10} M_\odot$ at $z = 0$.

8.6.2. *Filamentary gas accretion: Cold vs. hot modes*

Once the halo mass is large enough to be able to accrete, we must determine its fate. The first works to do this assumed spherically symmetric accretion that resulted in

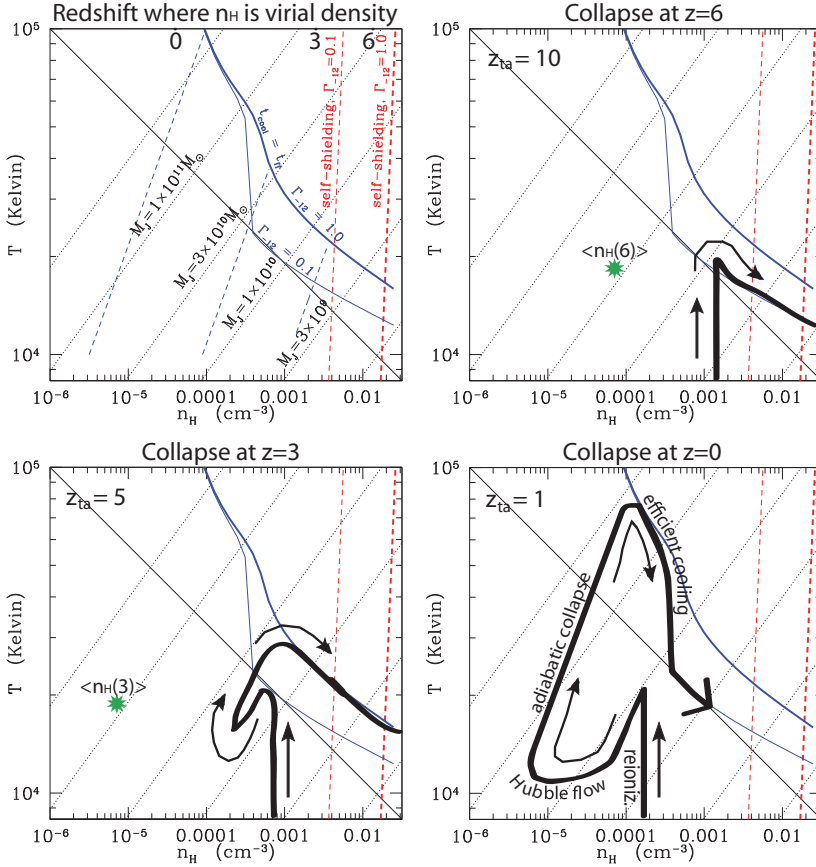


Fig. 8.10. A cartoon showing how diffuse gas evolves in the density–temperature plane as it accretes onto halos at various redshifts. In the first panel, the two solid blue lines show equilibrium temperatures for two different photoheating rates spanning the range expected for diffuse gas at these redshifts; dashed red lines show where self-shielding becomes important; a range of Jeans masses are shown as black dotted lines, and finally dashed blue indicates paths of constant entropy. The three following panels demonstrate, in a cartoon fashion, the path that diffuse gas takes in accreting onto three halos at three different times. The green star indicates the mean density at the collapse redshift. See text for discussion. Figure taken from [59].

shock-heating to the virial temperature of the halo, resulting in pressure supported gas in hydrostatic equilibrium [62]. The efficiency of gas cooling and star formation depended on the cooling time at that temperature and provided a broad-brush picture of how effectively halos of various masses were able to form stars [63]. Analytic arguments most fully developed in Ref. [64], suggested that in some halos the cooling would be strong enough to entirely prevent shock formation and so invalidate the assumption of hydrostatic equilibrium.

Numerical simulations have demonstrated that the situation is more complicated. An example is shown in Fig. 8.11 for a $10^{12} M_{\odot}$ halo at $z = 2$, extracted

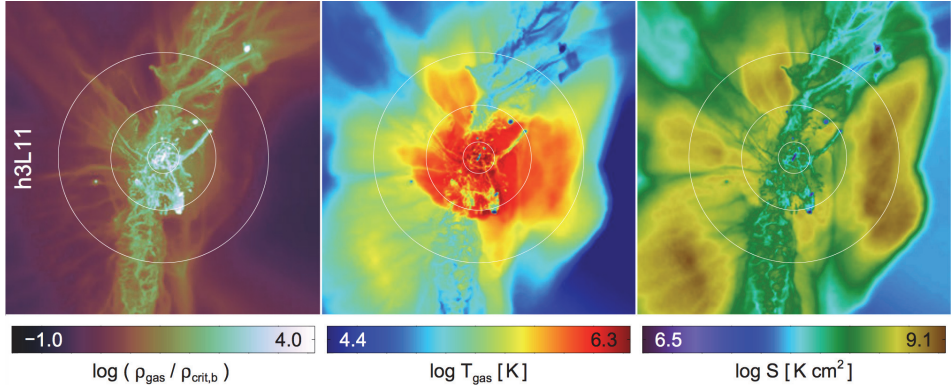


Fig. 8.11. Mass-weighted projections of gas density, temperature and entropy from the simulation of a $10^{12} M_{\odot}$ halo at $z = 2$ using the AREPO moving-mesh code. The white concentric circles show 0.15, 0.5 and 1.0 times the virial radius. Figure taken from [61].

from a set of zoom-in simulations designed to examine the circumgalactic gas at high-resolution, using the AREPO moving-mesh hydro code [61]. This image shows many interesting features typical of such flows: along some directions, there is a filamentary high-density inflow, which has low temperature ($T \lesssim 10^{5.5} \text{ K}$) as it goes through the virial radius. In other directions, the inflow is smooth and a clear accretion shock can be seen just past the virial radius. This shock shows a mild density increase, but much larger temperature and entropy increases.

This dichotomy between a cold (filamentary) mode of accretion, with a higher density but low covering fraction, and a hot (smooth) mode of accretion with lower density but covering more solid angle was pointed out by Ref. [65] and has been suggested to play a key role in galaxy regulation. The general principle is that cold mode accretion is much more likely to accrete directly onto the central galaxy and form stars, while gas which has been shocked-heated to the virial radius is easier to keep from cooling and forming stars. Indeed, higher mass halos at lower redshift tend to have a higher accretion rate in the hot mode, perhaps providing a natural explanation for their star forming quiescence [66]. The details of the interaction between these accretion modes and star formation remain poorly understood and more recent work has tended to focus on the importance of “ejective” feedback (that expels gas from the central star-forming galaxy) over “preventive” feedback that prevents hot gas from cooling in the first place.

The thermodynamics of accreting CGM gas is particularly challenging and our understanding of this process has evolved in the last few years. In Fig. 8.12, we show the distribution of mass accreted as a function of maximum temperature for a range of halo masses. This plot, from Ref. [67], contrasts two identical cosmological simulations evolved with the SPH code GADGET (on the right), and a moving mesh code AREPO (on the left). The maximum temperature of the fluid element is determined either as the maximum temperature of the SPH particle, or using

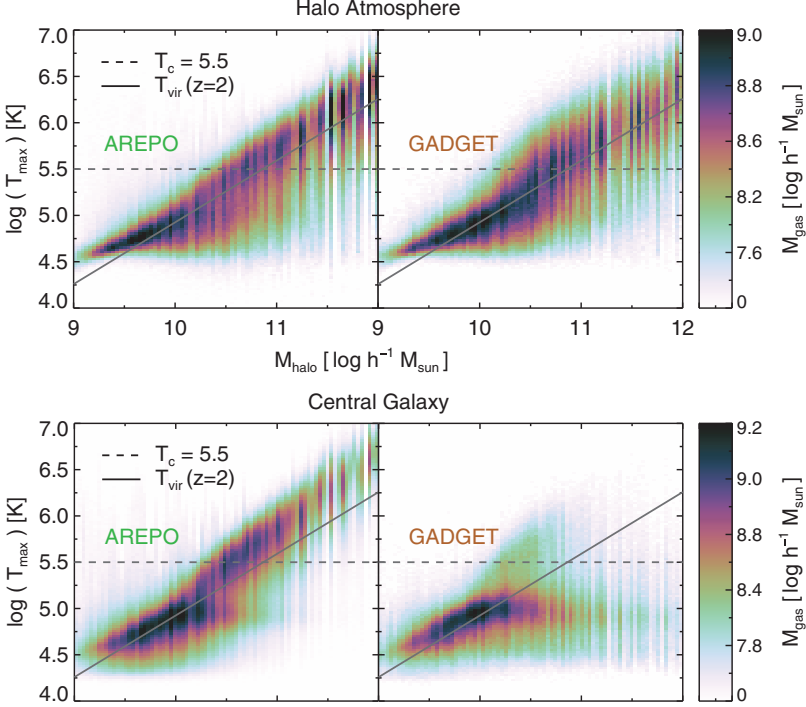


Fig. 8.12. The mass-weighted distribution of past maximum temperature for gas accreted onto central galaxies as function of halo mass at $z = 2$. The top panel shows the maximum temperature distribution for gas accreted past the virial radius, while the bottom panel shows the distribution for gas accreted onto central galaxy. The left panels use the moving-mesh code AREPO, while the right use the SPH code GADGET. Solid lines show the virial temperature at $z = 2$ and dashed lines highlight the typical temperature demarcation ($10^{5.5}$ K) between cold and hot flows. Figure taken from Ref. [67].

a tracer particle for the mesh code [68]. The top panel provides the maximum temperature for gas accreted past the virial radius (on to the halo atmosphere). We see that the temperature distribution roughly follows the virial temperature of the halo of that mass, but with a long tail to colder temperatures — these are the cold flows (and are more prominent with the usual fixed temperature cutoff of $10^{5.5}$ K, but are still present even when we use a virial temperature-based criterion). Note the good agreement between codes.

Therefore, the existence of cold flows into the CGM is well established; however, the bottom panel shows a similar distribution but for accretion onto the central galaxy itself. Here, there is a strong difference between codes, with SPH predicting that gas accretion onto the galaxy is primarily from cold mode gas; however, the mesh code indicates that nearly all of the gas is heated to the virial temperature before cooling and accreting. This occurs in part because the SPH code used here did not correctly model some fluid instabilities that prevented the mixing of hot

and cold gas — more recent work has corrected many of these problems [69]. This heating and mixing can be seen in Fig. 8.11 — the inflowing cold streams do eventually mix and shock heat at small radius — the vast majority of the gas within $0.15 r_{\text{vir}}$ is close to the virial temperature. Note also the increase in entropy of this gas (although it still remains much lower than smoothly accreted gas) — future work should look at the cold and hot flows through the lens of the entropy distribution.

Another interesting avenue of research into the dynamics of cold flows focuses on their angular momentum content. Recent work has demonstrated that the gas accreting in these flows has four times as much specific angular momentum as the dark matter accreting at the same time, a result that has recently been confirmed with a wide range of numerical methods [70]. This high angular momentum content is consistent with the idea that late accreting gas will preferentially build up the outer part of disk galaxies. Finally, we note that filamentary flows do not necessarily have to be cold, and simulations on both galaxy [71] and cluster scales indicate that gas filamentary accretion persists even when heated close to the virial temperature.

8.6.3. *Feedback and the CGM*

As the previous section demonstrates, the physics of CGM accretion are both very rich and challenging to model. This challenge is magnified by the addition of feedback from the central forming galaxy. Unfortunately, the impact of feedback is sufficiently poorly understood that no coherent picture has yet arisen. This arises in large part because our numerical models of feedback in galaxies remain poorly understood, although much recent progress has been made with the appearance of a number of different techniques which are able to accurately reproduce many of the observed properties of galaxies (see Chapter 6). Here, we briefly examine two parallel efforts to address the impact of feedback on the CGM: the first involves exploring a wide range of feedback models in simulations, while the second is more speculative and focuses more on the cooling properties of the gas. We will then turn to observational predictions and comparisons, which is probably the best current way to constrain models.

In Fig. 8.13, we show various CGM mass budgets for a set of simulations described in Ref. [72] in which they carried out eight different large-scale cosmological simulations with a wide variety of variations in feedback strength and methodology, including a Fiducial model which is tuned to reproduce many galactic properties. As the left panel demonstrates, the total CGM mass budget is relatively insensitive to the feedback methodology, while allowing large variations in the stellar and dense, cold gas components. However, this rosy simplicity falls apart when the detailed multiphase nature of the gas is examined, as the right panels demonstrate. The metal content of the CGM is similarly very strongly dependent on the strength of feedback. As we will show in the following section, on observations, while CGM

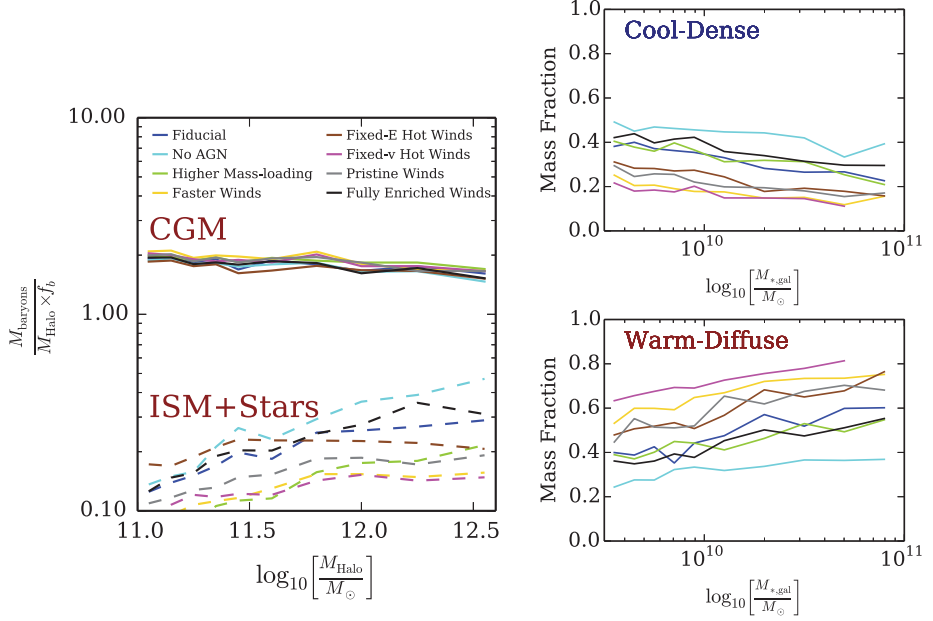


Fig. 8.13. The left panel shows the relative fraction of baryons in the CGM (solid lines, here taken to be within three virial radii) and in the galactic component (dashed) for a variety of different feedback methods in simulated halos with a wide range of (virial) masses, all at $z = 2$. The right panel shows a breakdown of the CGM mass content, showing two phases (cool-dense: $T < 10^5$ K and $n_H > 10^{-3} \text{ cm}^{-3}$ and warm-diffuse: $T > 10^5$ K and $n_H < 10^{-3} \text{ cm}^{-3}$) as a function of (stellar) mass. Figure taken from Ref. [72].

observational probes are still in their infancy, they already provide constraints that are difficult to match with these models.

An alternative and completely different approach to understanding the properties of gas halos has recently been proposed in Ref. [73], building on models which successfully describe the cooling gas in X-ray clusters as being in precipitation balance. That is, AGN heating operates to heat the gas (in a statistical sense) such that it is marginally stable to thermal instability. In detail, a feedback loop is set up in which the gas cools below the precipitation criterion, causing cool clumps to condense out and accrete onto the central black hole, triggering AGN events which heat the gas above the critical boundary. Simulations have found this critical boundary to be well described by the requirement that the local cooling time of the gas be 10 times the dynamical time ($t_{\text{cool}} \approx 10 t_{\text{dyn}}$). In Ref. [73], this model was extended to the CGM of galaxies, showing that if star formation came from gas condensing out of the CGM, many observed galactic scaling properties were naturally reproduced, including the mass-metallicity relation, the stellar-mass-halo-mass relation, and the correlation between the black hole mass and the stellar mass (for large galaxies). Although the model is still very simple, with many assumptions, more work along lines such as these seems warranted.

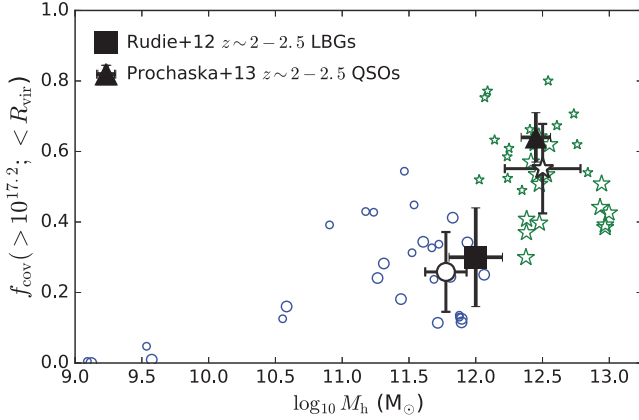


Fig. 8.14. The open symbols show the covering fraction for Lyman-limit absorbing systems ($N_{HI} > 10^{17.2} \text{ cm}^{-2}$) within the virial radius of a set of simulated systems at $z \sim 2-2.5$, compared to observed covering fractions, shown as filled black symbols (open black symbols are averages of the simulations for ease in comparison). Figure taken from [74].

8.6.4. Observations of the CGM

The CGM is very challenging to observe, due primarily to its very low density ($n_H \sim 10^{-4} \text{ cm}^{-3}$, or lower); however, its relatively large size can result in large column densities and hence absorption diagnostics in bright background systems (typically quasars). Much observational work has been carried out at high and low redshifts (too much to summarize here), see Ref. [75] for a recent review on the lower-redshift side, and Ref. [74] for a more detailed comparison to simulations.

Figure 8.14 shows the covering fraction for Lyman-limit HI systems (i.e., those with $N_{HI} > 10^{17.2} \text{ cm}^{-2}$) at $z = 2$ for a set of simulated systems with a range of halo masses (from Ref. [74]), compared to high-redshift absorption lines around a compilation of Lyman-break galaxies and even more massive galaxies hosting quasars. The good agreement seen here, which requires some form of feedback to achieve (in this case, based on the FIRE simulations), has also been found in other large-scale simulations, such as Illustris and EAGLE [76]. This indicates that the distribution of relatively dense gas (which gives rise to the relatively large column densities probed here) is well reproduced in the CGM at high redshift.

Probing the absorption in the CGM at low-redshift is more challenging, as it generally requires UV spectroscopy. However, recent advances using the COS spectrograph on HST have provided a wealth of data [78] to probe the gas conditions, even out to low density. This has driven a large number of groups to compare to this (and related) data, which includes absorption properties for hydrogen as well as a range of metal ions, with ionization potentials ranging from a few to hundreds of eV. These different ions probe a range of gas temperature and ionization states, ranging from MgII, which is a good tracer of neutral gas, up to OVII which is a probe of gas with $T \gtrsim 10^6 \text{ K}$.

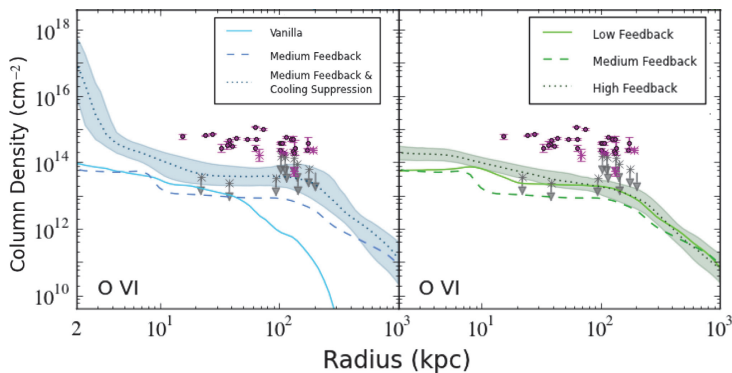


Fig. 8.15. The predicted OVI column density as a function of radius from a suite of simulations of a Milky-Way mass halo at $z = 0.2$ using different feedback prescriptions. Colored symbols with error bars and gray arrows are observations compiled from COS observations. Figure taken from [77].

One particularly interesting ion is OVI, which can be produced by photoionization in hard sources, but is more commonly seen in gas with temperatures close to $10^{5.5}$ K. This ion is observed to large projected distances in background quasars and has been challenging for many simulations to match. For example, in Fig. 8.15, we show the predicted OVI column density as a function of distance from a simulated $10^{12} M_{\odot}$ halo at low redshift, showing the systematic under-prediction compared to observations. This result has been explored in more detail in large-scale simulations with feedback prescriptions set to match many galaxy properties, and it is found that this disagreement appears to be quite robust and difficult to reconcile even with quite large changes in feedback prescriptions [79, 80].

8.7. Diffuse gas: Concluding remarks

We conclude this chapter with a few comments on the role that diffuse gas theory and observations will play in the coming years. First, as we have tried to convey, the basic theory for the ionization, heating and cooling of diffuse gas is generally in a good shape — this is particularly true for the IGM far from galaxies, where the ionizing background is the primary uncertainty. Closer to galaxies, in the CGM, the situation is much more uncertain, mostly due to the challenge in modeling feedback in galaxies, but also because our current generation of numerical methods tends to focus their efforts on the dense gas in galaxies. This is true of AMR, SPH and moving-mesh codes. Indeed, it is possible (and even likely) that a lot of CGM physics is operating on scales well below those of our current generation of simulations — an interesting recent suggestion is that the multiphase gas may exist at very small (sub-pc) scales [81]. An additional uncertainty is in the range of physical process explored. Most cosmological simulations discussed above have

treated gas in the hydrodynamical limit; however, magnetic fields may be important and even cosmic-rays have recently been suggested as an important player in the CGM [82]. In any case, it is clear that numerical models of diffuse gas will play a key role in the coming years.

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Chapter 9

Computational Modeling of Galaxy Clusters

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Galaxy clusters are the largest gravitationally bound objects in the universe, whose formation and evolution are driven by dark matter and dark energy. Recent multiwavelength observations have provided unprecedented insights into the structure and evolution of dark matter, gas, and stars from their cores to the virialization region in the outskirts of galaxy clusters. In order to realize the statistical power of upcoming cluster surveys, it is critical to improve our understanding of still uncertain cluster astrophysics. Given that clusters are nonlinear collapsed systems, N -body and hydrodynamic simulation is the method of choice for modeling the dynamics of dark matter, gas, and stars in their full complexity during the hierarchical build-up of structures. In this chapter, we will review recent advances in computational modeling of galaxy clusters formation with highlights on both successes and challenges.

9.1. Introduction

Clusters of galaxies are the largest gravitationally bound objects in the universe held together by gravity. The formation and growth of these magnificent objects are driven by dark matter (DM) and dark energy — the enigmatic but energetically dominant components of the universe. At the same time, the most massive black holes and galaxies form and grow at their centers through the complex interplay of gas and star formation over cosmic time, making them fascinating astrophysical objects and laboratories for studying galaxy formation and structure formation.

The majority of the baryonic mass in clusters resides in the X-ray emitting intracuster medium (ICM), which also leaves imprints in the cosmic microwave background (CMB) radiation. Modern X-ray observations with *Chandra* and XMM-*Newton* allow us to study the properties of the ICM with unprecedented detail and accuracy. Their superb spatial resolution and sensitivity enable resolved, accurate X-ray brightness and temperature maps from cores to the virialization region in the outskirts of galaxy clusters. Radio and gamma-ray observations, on the other hand, provide insights into nonthermal processes associated with magnetic field and cosmic rays in the ICM, while optical and infrared observations provide information about cluster member galaxies as well as the mass distribution in galaxy clusters through gravitational lensing effect.

By using clusters of galaxies as cosmological probes, modern astronomical observations have significantly constrained the picture of how the structure forms and evolves in the universe as well as tightened constraints on the nature of mysterious DM and dark energy. Cluster-based cosmological tests include cluster counts and their evolution with redshift [1–4], spatial distribution [5], and the angular-diameter distance measurements [6, 7]. Detailed observations of merging clusters provide unique insights into the physics of the intracuster plasma [8–10] and provide key evidence for the existence and properties of DM [11, 12]. However, all cosmological applications of clusters, at least to a certain degree, rely on solid understanding of the physics of their formation.

Since galaxy clusters are nonlinear collapsed systems, cosmological simulations are the method of choice for their theoretical studies. Modern cosmological simulation codes based on N -body and hydrodynamics techniques can follow the formation and evolution of DM and gaseous baryonic components in its full complexity through the hierarchical build-up of structures starting from the well-defined cosmological initial conditions. Yet, more realistic modeling of clusters requires inclusion of additional baryonic processes. For example, to model formation of cluster galaxies, we must, at the very least, treat energy dissipation due to radiative losses by baryons and conversion of gas into stars. In addition, any feedback in the form of energy injection and metal enrichment from supernova winds [13, 14] and active galactic nuclei (AGN) [15–17], and injection of cosmic rays at large-scale shocks accompanying cluster formation [18] can affect the thermodynamics of the ICM. Although our understanding of details and relative importance of these processes still remain uncertain, numerical simulations with specific assumptions about them are highly predictive and make models falsifiable. As such, by comparing the results of numerical simulations to observations, we can learn a great deal about astrophysical processes and their role in cluster formation.

We begin by outlining a simple theoretical framework in Section 9.2. We will then discuss key results from N -body and hydrodynamic simulations of galaxy cluster formation in Section 9.3. Effects of magnetic field, cosmic rays, thermal conduction, and plasma physics are discussed in Section 9.4. We conclude with a discussion of outstanding challenges and future prospects in Section 9.5.

9.2. Theoretical framework

In the paradigm of cosmological structure formation, gravitationally bound halos form at the peaks of the primordial density field as DM and baryons undergo nonlinear gravitational collapse (see Chapters 5 and 6 for more detailed discussions). DM, being collisionless and dissipationless, conserves its orbital energy, remaining in an extended dispersion-supported profile, with overlapping inward and outward moving orbits. By contrast, gas collides, shocks, mixes, and eventually dissipates energy via radiative cooling, causing it to collapse to the minimum of a halo's potential well and seed the formation of stars and galaxies.

9.2.1. Self-similarity

In the current hierarchical structure formation model, galaxy cluster of mass M at redshift z forms from gravitational collapse of the primordial cosmological density perturbation, when its linear density fluctuation $\delta(M, z)$ reaches the collapse threshold $\delta_c = 1.686$. Since the primordial density perturbations are well characterized by the Gaussian distribution, properties of galaxy clusters are uniquely characterized by its density peak height, $\nu(M, z) \equiv \delta_c / \sigma(M, z)$, where $\sigma(M, z)$ is the characteristic linear density fluctuation smoothed over mass scale M at redshift z .

The mass of a DM halo is commonly defined using a spherical overdensity of matter with respect to a reference density as

$$M_\Delta \equiv \frac{4\pi}{3} \Delta \rho_{\text{ref}}(z) R_\Delta^3, \quad (9.1)$$

where R_Δ is the radius within which we compute the enclosed mass. Two common choices of the background density ρ_{ref} are the critical density, $\rho_c(z) \equiv 3H_0^2 E^2(z) / (8\pi G)$, and the mean matter density, $\rho_m(z) = \rho_c(z) \Omega_m(z)$, in the standard Λ CDM spatially flat cosmological model, where $E^2(z) \equiv \Omega_m(1+z)^3 + \Omega_\Lambda$, $\Omega_m(z) = \Omega_m(1+z)^3 / E^2(z)$, and Ω_m (without the explicit z -dependence) refers to the present-day mass density fraction of the universe. The reference overdensity Δ is usually chosen to be a value close to $18\pi^2 \approx 178$, which corresponds to the virial overdensity in the flat matter dominated, Einstein-de Sitter universe ($\Omega_m = 1 - \Omega_\Lambda = 1$). In the more realistic flat Λ CDM model, the virial overdensity varies with redshift [19]. Note also that the spherical overdensity mass definition can lead to a spurious *pseudo-evolution* of halo mass simply due to redshift evolution of the reference density, even if its physical density profile remains constant over time [23], which must be accounted for when making phenomenological links between galaxies and DM halos as well as for models of galaxy evolution.

On large scales, the majority of the baryonic component is in the form of X-ray emitting ICM and is expected to follow the distribution of the gravitationally dominant DM. The self-similar model predicts that cluster gas profiles for a given mass (or peak height) appear *universal* when they are scaled with respect to the reference background density of the universe [24]. For example, the gas density is

scaled using the mean cosmic baryon overdensity, defined as $\rho_{\text{gas},\Delta} \equiv f_b \Delta \rho_{\text{ref}}(z)$, where Δ is the redshift independent chosen overdensity, $\rho_{\text{ref}}(z)$ is the reference mass density of the universe at redshift z , and $f_b \equiv \Omega_b/\Omega_m$ is the cosmic baryon fraction. Similarly, other quantities, such as temperature, pressure, entropy, and velocity, can be normalized with appropriate scaling that depends on mass and redshift: $k_B T_\Delta \equiv GM_\Delta \mu m_p / (2R_\Delta)$, $P_\Delta \equiv \rho_{\text{gas},\Delta} k_B T_\Delta / (\mu m_p)$, $K_\Delta \equiv k_B T_\Delta / (\mu m_p \rho_{\text{gas},\Delta}^{2/3})$, and $V_{\text{circ},\Delta} \equiv \sqrt{GM_\Delta / R_\Delta}$, where G is the gravitational constant, m_p is the proton mass, k_B is the Boltzmann constant, f_b is the cluster baryon fraction, and $\mu \approx 0.59$ to be the mean particle weight of the fully ionized ICM. For the cases where the reference background density is set to the critical or the mean density, we set $\Delta = \Delta_c$ or $\Delta = \Delta_m \equiv \Delta_c / \Omega_m(z)$, respectively.

9.2.2. Scaling relations

Scaling relations between the baryonic properties of clusters, such as X-ray temperature (T_X), X-ray luminosity (L_X), or the integrated Comptonization parameter (Y), and the total mass of galaxy clusters, are key to our understanding of clusters and their use in cosmology. For a more complete and detailed description of the predictions of the self-similar scaling model, we refer the reader to the discussion in [25], while we give a brief description for the most important relations below.

Cluster mass-temperature relation: The simplest model for these scaling relations relies on the assumption that cluster halos collapse in a self-similar fashion [26]. In this model, the temperature T , for example, scales with halo mass as

$$T \propto \frac{M}{R}, \quad (9.2)$$

where M denotes the mass within the radius R , and T is measured at R . If the halo mass is defined as a spherical overdensity mass (mass definitions such as $M_{500\rho_c}$ or $M_{500\rho_c}$ are commonly used for clusters), the above scaling relation can be expressed as

$$T \propto (\Delta_c \rho_c)^{1/3} M_\Delta^{2/3}. \quad (9.3)$$

Noting that Δ_c is a constant, but that the critical density evolves with $E^2(z)$, the evolution with redshift can be incorporated into the scaling relation as

$$T \propto [E(z) M_\Delta]^{2/3}. \quad (9.4)$$

Unfortunately, the $E^2(z)$ factor only accounts for the evolution of R due to the evolution of the ρ_c factor in Eq. (9.3), but *not* the pseudo-evolution of M_Δ . Thus, for a halo whose density profile remains constant, the scaling relation predicts that the temperature will increase with time without any particular physical reason.

X-ray scaling relations: The X-ray surface brightness is given by

$$S_X \propto \int n_e n_p \Lambda(T, Z) dV \propto \frac{1}{\mu_e \mu_p m_p^2} \int \rho_{\text{gas}}^2 \Lambda(T, Z) dV, \quad (9.5)$$

where $\Lambda(T, Z)$ is the cooling function which depends on temperature T and metallicity Z , μ_e and μ_p are the mean molecular weight of electrons and hydrogen, m_p is the proton mass, ρ_{gas} is the gas density, and V is the volume.

Sunyaev–Zel’dovich effect: The thermal Sunyaev–Zel’dovich (SZ) effect is a distortion in the CMB spectrum produced by the inverse Compton scattering of CMB photons off free electrons in dense structures such as clusters of galaxies [27, 28]. The change in the CMB specific intensity at a frequency ν caused by the thermal SZE is given by

$$\frac{\Delta I_\nu}{I_{\text{CMB}}} = f_\nu(x) g_\nu(x) y, \quad (9.6)$$

where $x \equiv h\nu/k_B T_{\text{CMB}}$, $f_\nu(x) = x(e^x + 1)/(e^x - 1) - 4$, and $g_\nu(x) = x^4 e^x/(e^x - 1)^2$. The magnitude of the thermal SZ signal is set by the dimensionless Comptonization parameter y ,

$$y \equiv \frac{k_B \sigma_T}{m_e c^2} \int n_e(l) T_e(l) dl, \quad (9.7)$$

which is proportional to the integrated line-of-sight thermal pressure of the ICM, and σ_T is the Thompson cross-section and c is the speed of light. The corresponding change in the CMB temperature is given by $\Delta T_\nu/T_{\text{CMB}} = f_\nu(x)y$. In the Rayleigh–Jeans limit ($\nu \ll 200\text{GHz}$), $\Delta T_\nu/T_{\text{CMB}} = -2y$ and $\Delta I_\nu = (2k_B \nu^2/c^2) \Delta T_\nu$.

Let us now consider the SZE signal arising from a cluster located at redshift z . The SZE flux integrated across the surface of a cluster is defined as the integrated Compton- y parameter Y_{SZ} :

$$Y \equiv \int_\Omega y d\Omega = \frac{1}{d_A^2(z)} \left(\frac{k_B \sigma_T}{m_e c^2} \right) \int_V n_e(l) T_e(l) dV, \quad (9.8)$$

and $d\Omega = dA/d_A^2(z)$ is the solid angle of the cluster subtended on the sky (the integral is taken over the volume of the cluster), $d_A(z)$ is the angular diameter distance to the cluster, dA is the area of the cluster on the sky, and dV is the cluster volume. Y measures the total thermal energy of a cluster. The thermal SZE signal is, therefore, linearly sensitive to gas mass $M_{\text{gas}} \equiv f_{\text{gas}} M$ and mass-weighted temperature T_m :

$$Y \propto f_{\text{gas}} M T_m \propto f_{\text{gas}} M^{5/3} E^{2/3}(z), \quad (9.9)$$

where f_{gas} is the gas mass fraction and M is the total cluster mass, where we inserted Eq. (9.4) into Eq. (9.9) to obtain the last expression.

9.3. Toward realistic modeling of galaxy cluster formation

While the spherical collapse model (discussed in Chapter 6) describes halo collapse in terms of instantaneous energetics, the actual physics of collapse is much more complicated, given that halos experience ongoing accretion, so they are almost never well-relaxed virialized systems. Given that clusters are nonlinear collapsed systems, numerical simulations are the method of choice for their theoretical studies. As described in Chapters 2 and 3, modern cosmological simulation codes based on N -body and hydrodynamics techniques are capable of following dynamical processes of DM and gas through the hierarchical build-up of structures (Figs. 9.1 and 9.2).

9.3.1. DM structures

9.3.1.1. DM density profiles

Collisionless DMs only of N -body simulations provide important insights into the structure of DM halos forming in the cold dark matter (CDM) scenario. The spherically averaged, radial density profiles within virialized halos of different masses can be described by an approximately universal profile [29–31]. One such form is the Navarro–Frenk–White (NFW) profile given by

$$\rho(r, z_i) = \frac{\rho_s}{(r/r_s)(1 + r/r_s)^2}, \quad (9.10)$$

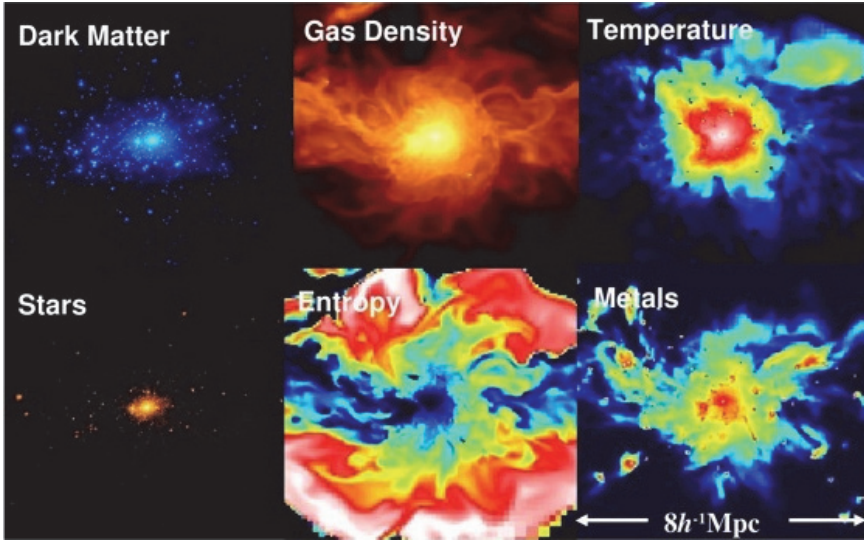


Fig. 9.1. Visualization of one of the present-day ($z = 0$) galaxy clusters simulated using the ART code, illustrating the rich thermodynamic and chemical structure captured by modern hydrodynamical cosmological simulations. From left to right, the distribution of DM, gas density and entropy (top) and stars, metallicity and temperature (bottom). The size of the region shown is $8h^{-1}$ Mpc (10% of the entire simulation volume).

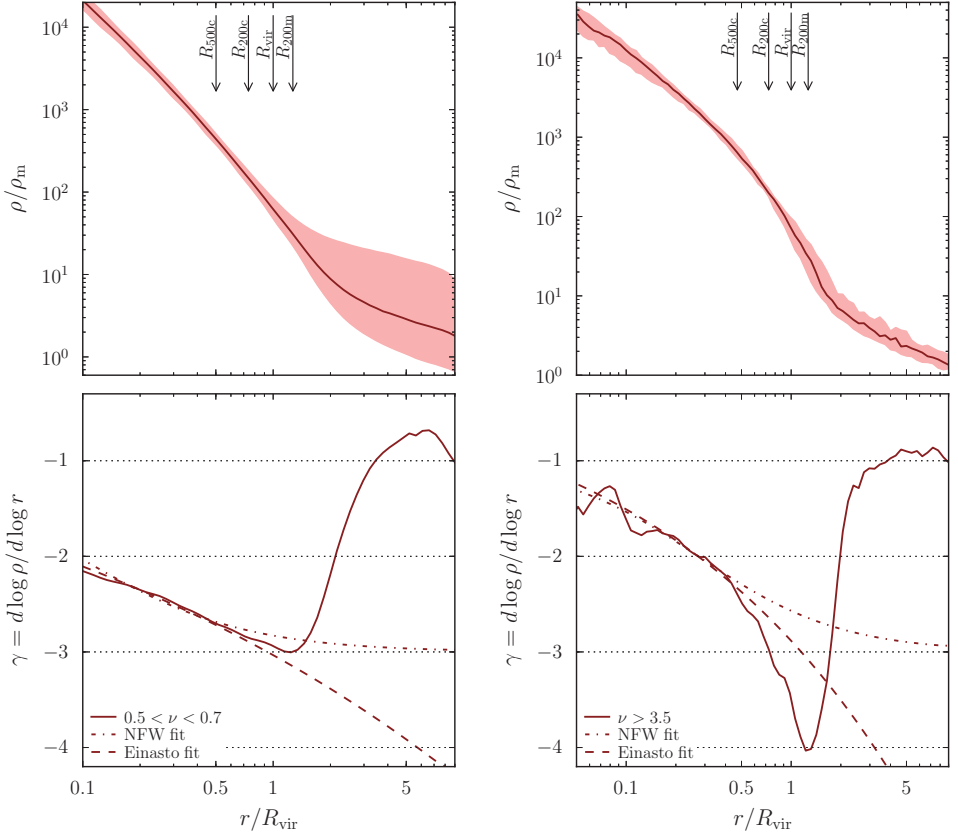


Fig. 9.2. Median DM density profiles of low-mass (top left panel) and high-mass (top right panel) halos at $z = 0$. The shaded bands indicate the interval around the median that contains 68% of the individual halo profiles in each ν bin. The vertical arrows indicate the position of various radius definitions. The shapes of the high- and low-mass profiles are noticeably different: the slope of the high- ν profile steepens sharply at $r \gtrsim 0.5 R_{\text{vir}}$, while the slope profile of the low- ν sample changes gradually until $r \approx 1.5 R_{\text{vir}}$, where the profiles of both samples flatten significantly. The bottom panels show the logarithmic slope profile of the median density profiles in the top panels, as well as the corresponding slope profiles for the best-fit NFW (dot-dashed) and Einasto (dashed) profiles. It is evident that the sharp steepening of the outer profile of the high- ν sample cannot be described by the NFW or Einasto profiles. Figure taken from Ref. [44].

where the scale radius r_s and the halo radius R_Δ are related by the concentration parameter $c_\Delta \equiv R_\Delta/r_s$. Note that this NFW profile has an inner asymptotic slope of -1 and an outer slope of -3 , and the concentration parameter is defined as the ratio of the outer virial radius and the radius at which the logarithmic slope is -2 . The concentration parameter is also known to depend on the formation time of the DM halo [30, 32] and/or a halo's mass assembly history [33, 34], giving rise to a tight relation between concentration, the shape of the profile at any given time, and the mass assembly history (MAH) of the main halo progenitor prior to

that time [34–36]. The MAH depends on the amplitude and shape of the initial density peak [37], which, in turn, depend on the mass scale of the peak as well as on the parameters of the background cosmological model. Thus, halo concentrations depend on mass, redshift, and cosmological parameters [30, 35, 36, 38–43].

Although nonbaryonic DM exceeds baryonic matter by a factor of $\Omega_{\text{dm}}/\Omega_{\text{b}} \approx 6$ on the average, the gravitational field in the central regions of galaxies is dominated by stars. In the hierarchical galaxy formation model, the stars are formed in the condensations of cooling baryons in the halo center. As the baryons condense in the center, they pull the DM particles inward, thereby increasing their density in the central region. The response of DM to baryonic infall has traditionally been calculated using the model of adiabatic contraction [45], which has also been tested and/or calibrated numerically using both idealized [46, 47] and cosmological simulations [48–51].

Recent work by Ref. [44] reported significant deviations from previously proposed fitting formulae at radii $r \gtrsim 0.5R_{200\text{m}}$. Specifically, they showed that halos that rapidly accrete mass exhibit a sharp steepening of their profile slope at $r \gtrsim 0.5R_{200\text{m}}$, with the maximum absolute value of the slope increasing with increasing mass accretion rate. The steepest slope of the profiles occurs at $r \approx R_{200\text{m}}$, and its absolute value increases with increasing peak height or mass accretion rate, reaching slopes of -4 and steeper. The outermost density profiles at $r \gtrsim R_{200\text{m}}$ are remarkably self-similar when radii are rescaled by $R_{200\text{m}}$. This self-similarity indicates that radii defined with respect to the mean density are preferred for describing the structure and evolution of the outer profiles. However, the inner density profiles are most self-similar when radii are rescaled by $R_{200\text{c}}$.

9.3.2. X-ray emitting ICM

Clusters are largely regular objects, exhibiting tight correlations between global properties of their various components that are expected from self-similar (i.e., gravity only) collapse and are confirmed in simulations. However, there are also important deviations from this simple picture due to the effects of nongravitational processes, such as radiative cooling and star formation in member galaxies, which play an important role in shaping the observable properties of galaxy clusters. Despite recent progress in theoretical and computational modeling of galaxy cluster formation, a variety of nongravitational effects are not yet well understood.

9.3.2.1. ICM profiles

Hot X-ray emitting ICM constitutes about 10% of the total gravitating mass of galaxy clusters and is the dominant baryonic component. If the gravitational potential of a cluster is static, then the gas would eventually settle into hydrostatic equilibrium (HSE) with the density and temperature isosurfaces aligned with the equipotential surfaces. If in addition the potential is spherically symmetric, then all

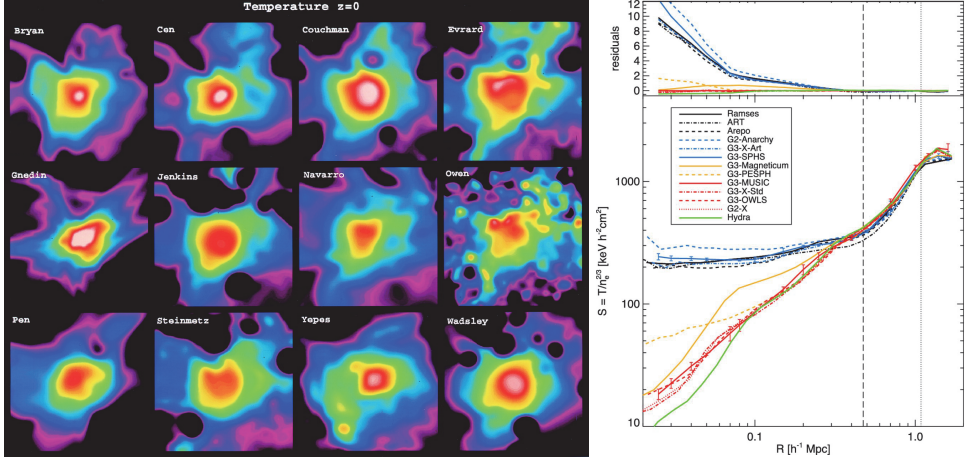


Fig. 9.3. *Left panels:* Integrated, mass-weighted gas temperature of a simulated cluster at $z = 0$ from the Santa Barbara Cluster Comparison project. The images, covering the inner 8 Mpc of each simulation cube, have been smoothed using the standard Gaussian filter of 250 kpc half-width. Taken from [52]. *Right panel:* Radial variation of the gas entropy, defined as $S = \ln(T/\rho)$ of the simulated cluster at $z = 0$ from the nIFTy galaxy cluster simulations project. The different lines show the result of the 13 different simulations, showing the discrepant results in the central entropy profile performed by different (e.g., classic SPH vs. AMR mesh) codes. Figure taken from Ref. [53].

gas thermodynamic properties (e.g., density and pressure) are functions of radius only, i.e., the ICM is homogeneous within a narrow radial shell.

In order to ensure the numerical results are accurate and robust, it is critical to perform a detailed comparison of hydrodynamical codes which simulate the formation and evolution of a galaxy cluster. A pioneering comparison was performed within the Santa Barbara Cluster Comparison Project [52] (see the left panel of Fig. 9.3). In this project, 12 different groups, each using a code either based on the SPH technique (seven groups) or on the grid technique (five groups), performed a nonradiative simulation of a galaxy cluster from the same initial conditions. A more recent comparison project, the so-called nIFTy galaxy cluster simulations [53], included modern SPH implementations as well as the moving mesh code *AREPO* in addition (see the right panel of Fig. 9.3). A similar agreement over large ranges was obtained for many of the ICM profiles (such as the density, temperature, and entropy profile) in both studies, as shown in the right panel of Fig. 9.3). Both studies found significantly larger differences between mesh-based codes and classical particle-based codes to be present for the inner part of the profiles. However, as shown in [53], particle-based codes which include an explicit treatment of mixing are giving results very similar to grid-based codes. It is worth mentioning that the treatment of additional physical processes, such as star formation and SNe/AGN feedback, would have even more significant impact on the ICM properties [54].

9.3.3. Baryonic physics

One of the key challenges in computational modeling of galaxy cluster formation lies in modeling of cluster galaxies and impacts of galaxy formation physics on clusters' observable properties. Since the dynamic range involved in this problem is still very far from reachable even by the most powerful computers today, making progress on this problem requires development of a subgrid model (i.e., *effective theory*) on a variety of scales that must be patched together. Modern hydrodynamical cosmological simulations include galaxy formation processes critical to various aspects of galaxy formation: star formation, metal enrichment and energy feedback by supernovae and AGN, self-consistent advection of metals, metallicity-dependent radiative cooling and UV heating due to cosmological ionizing background.

9.3.3.1. Gas cooling, star formation, and stellar feedback

Recent comparisons of numerical simulations and X-ray and microwave observations have been particularly instrumental in characterizing and controlling systematic uncertainties associated with still poorly understood astrophysical processes. For example, although the physical mechanisms that govern cluster cores are still uncertain, the current generation of cosmological simulations is capable of reproducing the observed properties of the ICM well at large radii, $0.2 < r/R_{500} < 1$ [56] (see Fig. 9.4). The outer regions of galaxy clusters ($r \sim R_{500}$) can thus be used to obtain accurate cluster mass measurements. In order to gauge the role of galaxy

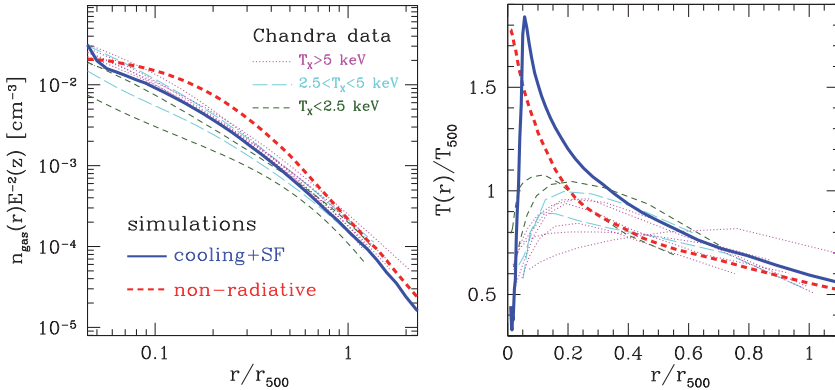


Fig. 9.4. Comparison of the ICM profiles in relaxed clusters in cosmological cluster simulations and the *Chandra* sample of [55] in the local universe at $z \approx 0$. The panels show the gas density (left) and gas temperature (right). Thick solid and dashed lines show the mean profiles in the cooling and star formation and nonradiative simulations, respectively, while the observed profiles are shown by the thin dotted, long-dashed, and short-dashed lines for the systems with $T_X > 5$ keV, $2.5 < T_X < 5$ keV, and $T_X < 2.5$ keV, respectively. Note that at $r \gtrsim 0.1r_{500}$, the profiles of the CSF simulations provide a better match to the observed profiles than the profiles in the nonradiative runs, but the CSF runs (without AGN feedback) are still strongly inconsistent with the observed profiles of cluster cores. Figure taken from Ref. [56].

formation in shaping properties of the ICM, one compares the ICM profiles of simulated clusters with varying input physics. The first set of simulations is performed in nonradiative regime and hence does not reach high densities nor form stars. The second set of simulations includes the physics of galaxy formation: gas cooling, star formation, metal enrichment and thermal feedback due to the supernovae, which we denote as “CSF” run hereafter. By comparing the simulated profiles in these sets of simulations to those of observed clusters, we can assess the role of galaxy formation physics on the ICM properties.

9.3.3.2. *AGN feedback*

Black holes (BHs) also play an essential role in the formation and evolution of galaxy clusters and their ICM. However, observations of AGN indicate that gas accretion onto BHs and AGN feedback are complex processes, which are not yet fully understood [57–59]. There is evidence for two distinct phases of AGN activity and feedback: the radio-mode and the quasar-mode. The radio-mode is characterized by large radio jets generating hot X-ray cavities [60, 61], whereas in the quasar-mode, the emission is dominated by the accretion disc, which is visible as the so-called blue bump in the spectrum of quasars and Seyfert galaxies [62, 63].

Although including AGN feedback in cosmological simulations results in substantial improvement of the predicted ICM properties compared to observations [65–68], it is still quite challenging for cosmological simulations to reproduce the diverse population of cool core and noncool core systems and their internal properties. Only recently, Ref. [64] were able to produce consistent cool core and noncool core in simulations. Here, the combination of an advanced modeling of the BHs and its associated feedback [69] in combination with the capability of describing gas mixing in an improved SPH method [70] results in reproducing some key observational properties in cool core and noncool core systems. In these simulations, a fraction similar to the observed one shows clear cool core properties, with no entropy core in the center and steeper metal gradients while the rest show clear noncool core properties, harboring a similar entropy plateau in the center and a significantly shallower metallicity profile (see Fig. 9.5). Furthermore, these simulations indicate transformations between cool core and noncool core systems over quite short timescale and even at low redshift, in contrast to earlier suggestions that the diversity of such systems is set at early times.

9.3.3.3. *Scaling relations*

For the past three decades, such comparisons were used extensively to put constraints on the deviations of ICM thermodynamics from the simple self-similar behavior, described originally by Refs. [26, 71]. Observationally, it has long been known that the observed correlation of cluster X-ray luminosity, L_X , and spectral temperature, T_X , deviates significantly from the prediction of the self-similar model.

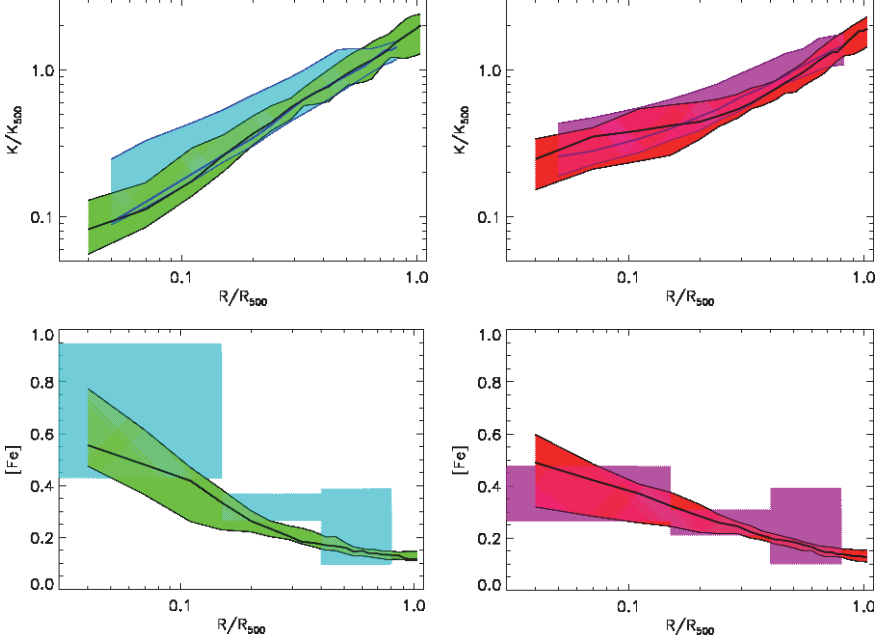


Fig. 9.5. Comparison of entropy (upper row) and metallicity (lower row) profiles of the ICM in cool core (right panels) and noncool core (left panels) clusters from simulations with AGN feedback (green and red) and observations, respectively. Figure taken from Ref. [64].

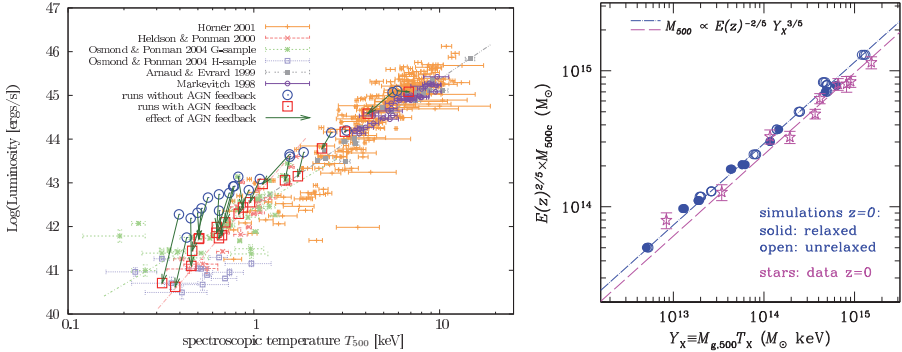


Fig. 9.6. Comparisons of $L_X - T_X$ [[65] left panel from [66]] and $Y_X - M_{500}$ [[103] right panel from [104]] relations for galaxy cluster from simulations and observations in the local universe.

The slope of the $L_X - T_X$ relation is significantly steeper than the slope predicted by the self-similar model [1, 72–76], and it steepens for the lowest mass clusters [77–79]. Deviations from self-similarity were shown to be the strongest in the cores of clusters [55, 74, 80] and were widely interpreted as evidence for preheating of the ICM by energy from supernovae and AGN feedback (e.g., [65, 71, 81–83, 87]; see also the left panel of Fig. 9.6) and/or the effects of gas cooling and condensation of

the gas accompanying formation of cluster galaxies (e.g., [89–91, 97]). However, the amount of gas that condenses out of the hot ICM in cosmological simulations due to gas cooling [92, 95, 98–100] was too large compared to the observed stellar mass in clusters [101, 102]. Thus, the X-ray measurements appear to be consistent with a large fraction of cooling gas, while the optical estimates of stellar mass indicate that this fraction is small.

One of the most important scaling relations, especially for cosmological application, is the observable–mass relations. A number of mass proxies have been invested in the literature, including X-ray luminosity (L_X), temperature (T_X), gas mass (M_g), integrated SZ signal (Y_{SZ}), using both observations and simulations. All scalings exhibit a high degree of regularity and tight correlations between the considered observables and total mass, but with varying degrees of sensitivity to the still poorly understood cluster astrophysics.

The right panel of Fig. 9.6 shows one example of X-ray proxy for the cluster mass, the X-ray pressure ($Y_X \equiv T_X M_g$), comparing the X-ray observable–mass relations of the CSF simulations and *Chandra* X-ray observations of nearby relaxed clusters. The mass proxy was derived from mock *Chandra* images of the simulated clusters and by analyzing them using a model and procedure used in real data analysis, and T_X was obtained by a single temperature to the spectrum extracted from the radial range of $[0.15–1]r_{500}$ (excluding emission from cluster core). Remarkably, the M_{500} – Y_X relation shows the scatter of only $\approx 7\%$, making it one of the most robust mass proxies known to date. The tightness of the M_{500} – Y_X relation and simple evolution are due to a fortunate cancellation of opposite trends in gas mass and temperature [103, 104]. The slope and redshift evolution of normalization for the M_{500} – Y_X relations are well described by the simple self-similar model [105, 106].

The M_{500} – T_X relation, on the other hand, exhibits a larger scatter of $\sim 20\%$ in M_{500} . Most of the scatter is due to unrelaxed clusters. The unrelaxed clusters also have temperatures biased low for a given mass because the mass of the system has already increased, but only a fraction of the kinetic energy of merging systems is converted into the thermal energy of gas due to incomplete thermalization during mergers [107, 108]. The slope and redshift evolution of the M_{500} – T_X relations are quite close to the simple self-similar expectation. Note that the M_{500} – M_g relation has a somewhat smaller scatter ($\approx 11\%$) around the best-fit power-law relation than the M_{500} – T_X , but its slope is significantly different from the self-similar prediction for the M_{500} – M_g relation due to the trend of gas fraction with cluster mass present for both the simulated clusters [109, 110] and for the observed clusters [55].

Note that the normalizations of the ICM scaling relations from simulated and observed clusters show the offset of about 10–15% due to the uncertainty associated with the hydrostatic mass estimate of galaxy clusters (see Section 9.3.4.3 for further discussion).

9.3.4. Beyond the spherical cows

So far, we have assumed that the gravitational potential of a cluster is both *spherically symmetric* and *static*, then the gas would eventually settle into HSE with the density and temperature isosurfaces aligned with the equipotential surfaces. Under these assumptions, all gas thermodynamic properties (e.g., density, temperature, and pressure) are functions of radius only, i.e., the ICM is homogeneous within a narrow radial shell. In reality, both X-ray observations and hydrodynamical simulations of galaxy clusters show that the gas is continuously perturbed as a cluster forms and the ICM is not perfectly homogeneous. Among plausible sources of the ICM inhomogeneities are nonsphericity of the gravitational potential, fluctuations of the potential, e.g., due to moving subhalos associated with galaxies or subgroups, low entropy gas clumps, presence of bubbles of relativistic plasma, turbulent gas motions and associated gas displacement, sound waves and shocks, etc. We will discuss our current understanding of the departures from the idealized model assumptions often adopted when analyzing and interpreting observations of galaxy clusters.

9.3.4.1. Shapes of DM and ICM

The CDM paradigm predicts that DM halos are generally triaxial and are elongated along the direction of their most recent major mergers [29, 112–122]. The degree of triaxiality is correlated with the halo formation time [119, 123, 124], suggesting that at a given epoch, more massive halos are more triaxial. For the same reason, triaxiality is sensitive to the linear structure growth function and is higher in cosmological models in which halos form more recently [125]. It is also well known that including baryons in simulations modifies the shapes of DM halos, especially in the case of significant gas dissipation associated with galaxy formation processes [126–134].

Figure 9.7, for example, illustrates that gas traces the shape of the underlying potential rather well outside the core, as expected in HSE, but the gas and potential shapes differ significantly at smaller radii [111]. These simulations further suggest that with radiative cooling, star formation and stellar feedback (CSF) intracuster gas outside the cluster core ($r \gtrsim 0.1r_{500}$) is more spherical compared to nonradiative simulations, while in the core, the gas in the CSF runs is more triaxial and has a distinctly oblate shape. The latter reflects the ongoing cooling of gas, which settles into a thick oblate ellipsoid as it loses thermal energy. In the CSF runs, the difference reflects the fact that gas is partly rotationally supported. In nonradiative simulations, the difference between gas and potential shape at small radii is due to random gas motions, which make the gas distribution more spherical than the equipotential surfaces. Results are similar for unrelaxed clusters, but with considerable scatter. In both CSF and nonradiative runs, gravitational potential is much more spherical than DM.

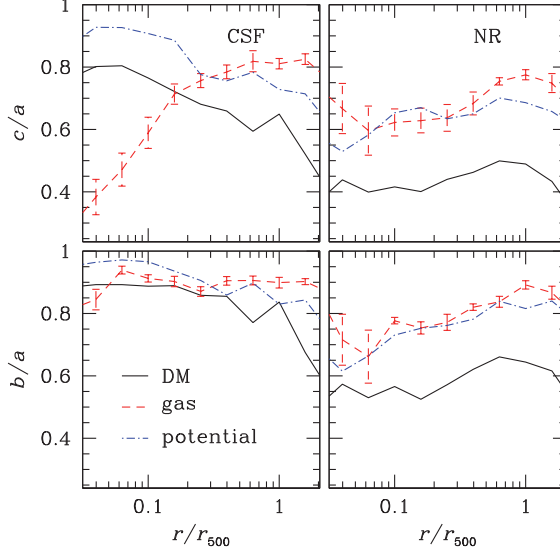


Fig. 9.7. Average ellipsoidal axis ratio profiles for the *relaxed* $z = 0$ clusters from the CSF run (left panels) and the NR run (right panels). The upper panels show the profiles for the short-to-long axis ratio c/a , and the bottom panels show the profiles for the intermediate axis ratio b/a . In all panels, the solid line corresponds to DM, the dashed line corresponds to gas, and the dot-dashed line corresponds to gravitational potential. The error bars show 1σ error on the mean axis ratio for gas. The magnitude of the errors on the mean axis ratios for gas is similar to those of DM and potential. Figure taken from Ref. [111].

9.3.4.2. Gas inhomogeneities

In the hierarchical structure formation model, clusters grow by accreting materials from the surrounding large-scale structure in their outer envelope. Hydrodynamical simulations predict that accretion and mergers are ubiquitous and important for cluster formation (see Video 6, page xiii), and the accretion physics gives rise to internal gas motions and inhomogeneous gas density distribution (“clumpiness”) in the ICM. Since the observed X-ray surface brightness profile (in Eq. 9.5) depends primarily on the square of gas density, the ICM density derived from X-ray observations could be biased by a clumping factor:

$$C \equiv \frac{\langle \rho_{\text{gas}}^2 \rangle}{\langle \rho_{\text{gas}} \rangle^2} \geq 1. \quad (9.11)$$

In X-ray analyses of galaxy clusters, it is commonly assumed that the ICM is not clumpy (i.e., a single phase medium characterized by one temperature and gas density within each radial bin, and hence $C = 1$). However, if the ICM is clumpy, the gas density inferred from the X-ray surface brightness is overestimated by $\sqrt{C(r)}$. In what follows, we investigate the clumping factor of the X-ray emitting ICM using hydrodynamical cluster simulations.

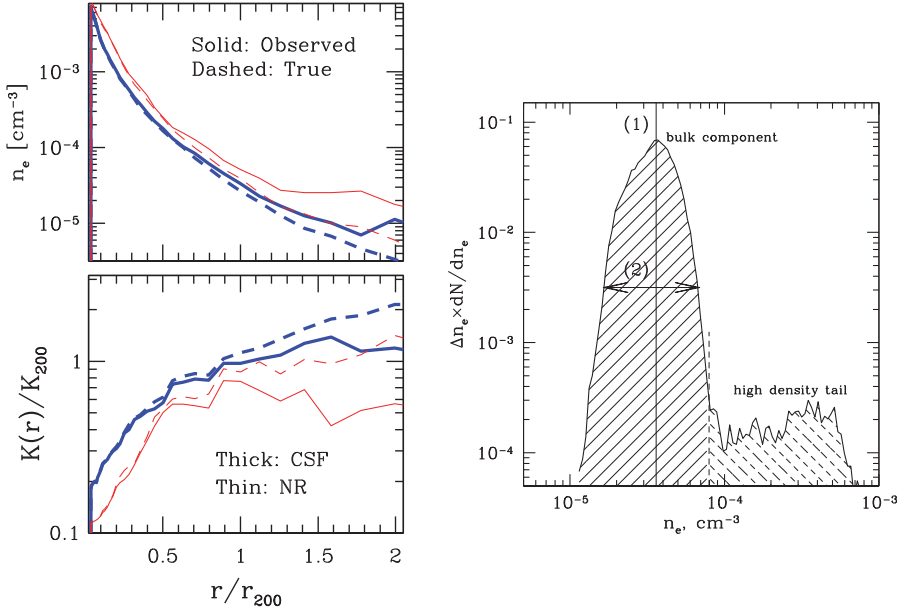


Fig. 9.8. *Left panels:* Effects of gas clumping on X-ray measurements of the ICM profiles. Gas clumping causes the overestimation of electron number density profile (top) and the flattening of the entropy profile (bottom) for gas with $T > 10^6$ K. Solid lines indicate observed profiles, while dotted lines indicate true profiles. Thick and thin lines correspond to CSF and NR runs, respectively. From [135]. *Right panels:* Sketch of ICM inhomogeneities. The solid curve shows the Probability Distribution Function of the density in a radial shell at $1.1\text{--}1.2r_{500}$ in one of the relaxed simulated clusters with gas cooling and star formation. The solid vertical line shows the median value of the density. The ICM is divided into two components (hatched regions): bulk, volume-filling component and high density inhomogeneities, occupying small fraction of the shell volume. The bulk component in the paper is characterized by two main parameters: (1) the median value of the density and (2) the width of the density distribution. The separation of the components is based on the width of the bulk component and the deviation of the density from the median value. Figure taken from Ref. [136].

Although the bias in the inferred ICM mass is moderate ($\lesssim 10\%$) in the high-pressured regions in the interior of galaxy clusters [137], gas clumping can become significant in the envelope of galaxy clusters ($r \gtrsim r_{200}$) and could serve as a major source of systematic bias in X-ray measurements of ICM profiles [135]. For example, gas clumping introduces the overestimation of the observed gas density and causes flattening of the entropy profile at large radius. This is illustrated in Fig. 9.8. The top-left panel shows that the clumping factor of the X-ray emitting gas ($T \gtrsim 10^6$ K) is $C \equiv \langle \rho_{\text{gas}}^2 \rangle / \langle \rho_{\text{gas}} \rangle^2 \sim 1.3$ at $r = r_{200}$, and it increases with radius, reaching $C \sim 5$ at $r = 2r_{200}$. In the bottom-left panel, the solid line indicates the true entropy profile, which is consistent with the self-similar prediction, $K \equiv T/n_e^{2/3} \propto r^{1.1}$ [138]. From the definition of entropy, the overestimation of gas density due to clumping causes an underestimation of the observed entropy profile by $C(r)^{1/3}$, suggesting

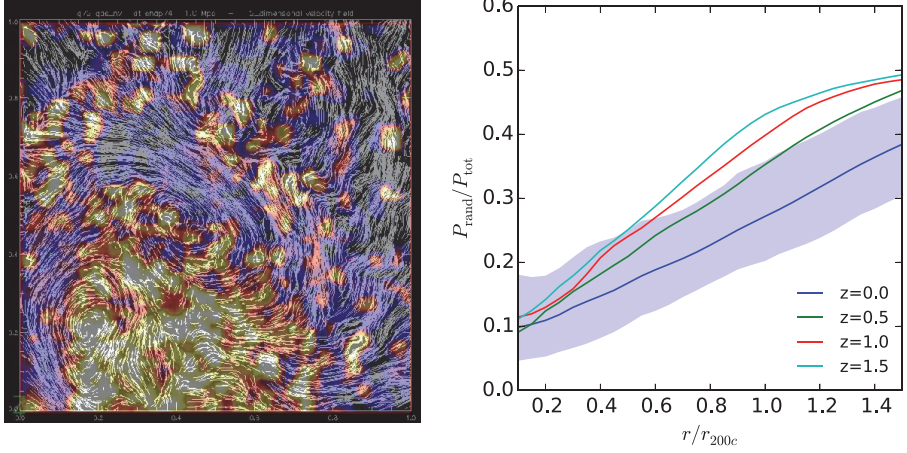


Fig. 9.9. *Left panel:* Gas velocity field in a slice through the central Mpc of a galaxy cluster simulation after subtracting the global mean bulk velocity of the cluster. The underlying color map represents the ratio of turbulent kinetic energy and total kinetic energy content of particles, inferred using the local velocity. From [140]. *Right panel:* Redshift dependence of the profile of nonthermal pressure fraction $P_{\text{rand}}/P_{\text{tot}}$, with radius scaled with respect to r_{200c} (top). The shaded regions denote the $1\text{-}\sigma$ scatter around mean at $z = 0$. Our fitting formula is overplotted in the dashed line. Figure taken from Ref. [108].

that gas clumping causes the flattening of the observed entropy profiles at $r \gtrsim r_{200}$ (see [139] for a review).

9.3.4.3. Turbulent and Bulk Motions

In the hierarchical structure formation model, clusters of galaxies form through a sequence of mergers and continuous mass accretion. These merging and accretion events generate a significant level of gas motions inside the cluster potential well, which eventually heats the gas through shocks or turbulent dissipation (see the left panel of Fig. 9.9). Hydrodynamical simulations of intracluster gas using both grid-based [107, 108, 142–145] and particle-based [140, 146, 147] methods have found that the intracluster gas motions generated in the structure formation process contributes significantly to the nonthermal pressure of the ICM. In addition to the structure formation process, turbulent gas motions can be generated in the cluster outskirts by the magnetothermal instability [148, 149] and in the cluster core by core sloshing [150–152], the heat buoyancy instability (HBI) [153] and/or energy injection from BHs and stars (see [154] for a review). Magnetic fields and cosmic rays may also contribute to the nonthermal pressure (see Section 9.4 for discussions). Residual acceleration of gas, apart from the nonthermal pressure, introduces an additional source of deviation from the HSE [108, 155, 156].

Understanding the nonthermal pressure in galaxy clusters is especially important because X-ray and SZ observations typically measure only the thermal pressure

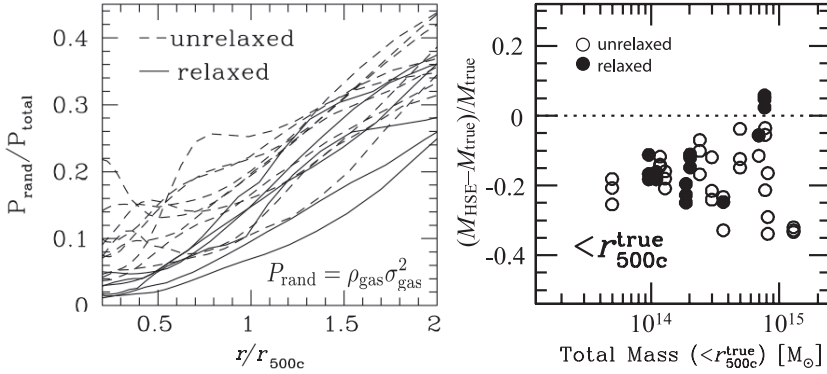


Fig. 9.10. *Left panel:* Ratio of pressure from random gas motions to total pressure as a function of radius [107]. Relaxed clusters are represented by solid lines while unrelaxed clusters are represented by dashed lines. *Right panel:* Hydrostatic mass bias defined as $(M_{\text{HSE}} - M_{\text{true}})/M_{\text{true}}$ at $r = R_{500}$ for simulated clusters at $z = 0$ [141]. Each cluster is viewed along three orthogonal projections, and clusters with relaxed and unrelaxed morphologies are indicated with filled and open symbols, respectively.

of the gas. Nonthermal pressure, if neglected, introduces biases in our physical understanding of the ICM profiles as well as the hydrostatic mass estimation. For example, the increasing kinetic energy fraction at larger radii leads to suppressed temperatures and flatter entropy profiles in cluster outskirts (see [139] for a recent review and references therein). Gas motions also contribute to the support against gravity which leads to biases in cluster mass estimates based on the assumption of HSE [141, 157–160]. The HSE mass bias is considered to be one of the primary sources of systematic uncertainties in the calibration of cluster observable–mass relations and cosmological parameters derived from clusters [161–163] (see Fig. 9.10). A large kinetic energy fraction in cluster outskirts also reduces the thermal SZ signal of individual clusters and the SZ fluctuation power spectrum [164–166], introducing additional uncertainties in cosmological inference from ongoing SZ surveys [167, 168]. Moreover, gas motions are thought to be responsible for dispersing metals throughout the ICM via turbulent mixing [169] and accelerating particles which gives rise to high-energy X-ray emission in clusters [170].

Despite the important role of gas motions in cluster astrophysics and cosmology, we know very little about them observationally. Several observations have provided indirect evidence for the intracluster gas motions: measurements of the magnetic field fluctuations in diffuse cluster radio sources [171–174], X-ray surface brightness fluctuations or pressure fluctuations inferred from X-ray maps [175–178], and the nondetection of resonant scattering effects in the X-ray spectra [179]. The HSE mass bias manifests itself as a systematic difference between the X-ray (or SZ) derived mass and the lensing mass of up to 30% [180–184], but see also [185].

Future observations of the X-ray emission lines are considered as the most promising method to measure turbulence velocities directly [186–188], and so far

the method has already provided a few upper limits in the cluster cores [189, 190]. However, these measurements are likely limited to the inner regions of a handful of nearby massive galaxy clusters [191]. Next generation X-ray missions, such as Athena+¹ and SMART-X², are necessary to extend such study for a cosmologically representative sample as well as higher redshift and lower mass groups and to provide fuller insights into the missing energy problem in galaxy clusters. In the future, high-resolution, multifrequency SZ observations (e.g., CARMA, CCAT, MUSTANG2) are sensitive to thermodynamics and velocity structures of the hot gas in the outskirts of galaxy clusters [192, 193].

9.3.4.4. Observations of cluster outskirts

Recent measurements by the Suzaku X-ray and Planck microwave satellites have pioneered the study of the hot gas in the ICM in cluster outskirts beyond R_{500} [196–199]. These measurements had unexpected results in both entropy and enclosed gas mass fraction at large radii. Entropy profiles from Suzaku data were significantly flatter than theoretical predictions from hydrodynamical simulations [195, 200] (see also the right panel of Fig. 9.11), and the enclosed gas mass fraction from gas

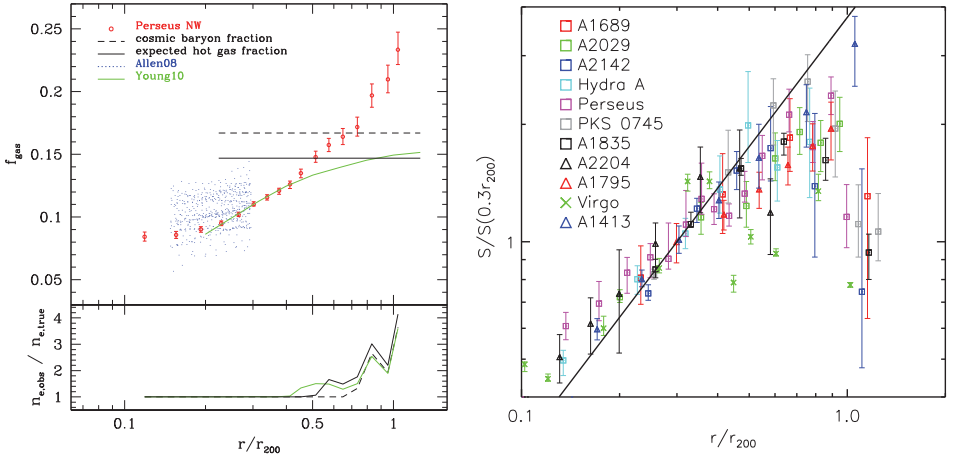


Fig. 9.11. Suzaku X-ray observations of the virialization region in the outskirts of galaxy clusters. *Left panel:* Observed gas mass fraction in Perseus exceeds the cosmic baryon fraction from WMAP7 data at $r \gtrsim 0.7R_{200}$ (top panel). The bottom panel shows by how much the electron density should be overestimated in each annulus due to gas clumping in order for the cumulative f_{gas} not to exceed the correspondingly colored curves in the plot above. Taken from [194]. *Right panel:* Observed entropy profiles of relaxed clusters are considerably flatter than the theoretically predicted relation of $K \equiv T/n_{\text{gas}}^{2/3} \propto r^{1.1}$ (indicated with a solid line) at $r \gtrsim 0.7R_{200}$. Figure taken from Ref. [195].

¹<http://www.the-athena-x-ray-observatory.eu>.

²<http://hea-www.cfa.harvard.edu/SMARTX>.

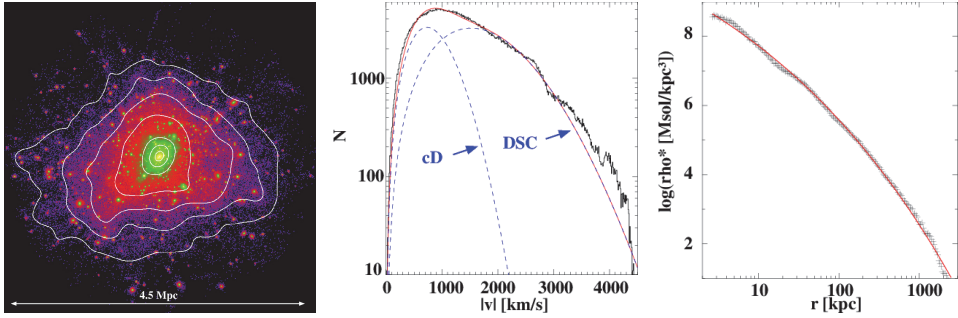


Fig. 9.12. Stellar density map of a simulated, massive galaxy cluster (color coded). The white contours show the diffuse stellar component plus the central galaxy (cD) after subtracting the stars from the other cluster member galaxies. *Middle*: Distribution of the stellar velocities for the DSC and the cD galaxy (black histogram) with a double Maxwellian fit (red line). *Right*: Radial stellar density profile of cD and DSC (black symbols) with a single Sérsic profile fit (red line). Figure taken from Ref. [207].

mass measurements of the Perseus cluster exceeded the cosmic baryon fraction [194, 201] (see also the left panel of Fig. 9.11). These results suggested that the measurements of the ICM in cluster outskirts may be complicated by (1) gaseous inhomogeneities in the X-ray emitting ICM that can cause an overestimation in gas density and flattening of the entropy profile at large radii [135, 136, 202, 203] and/or (2) contributions from the cosmic X-ray background [204, 205]. Recent deep *Chandra* observations of the outskirts of galaxy cluster Abell 132 have addressed both of these problems. First, the superb angular resolution ($\lesssim 1$ arcsec) allowed efficient point source removal and isolation of the cosmic X-ray background. Second, the long exposure time of 2.4 Msec enabled the detection of small-scale clumps and filaments, demonstrating that they dominate the X-ray emission from the cluster outskirts.

9.3.5. Stellar components in clusters

The stellar component of galaxy clusters (see Video 7, page xiii), although the least massive component, represents an important tracer of the MAH of the cluster. In addition, galaxy clusters reflect the most extreme environments to shape the evolution of individual galaxies which in turn significantly influence both thermodynamic and chemical properties of the ICM. While within the whole cluster, the cosmic baryon fraction given as the sum of the ICM and the stellar component is largely conserved, individual clusters show a wide spread of stellar and gas mass fraction, which therefore are anticorrelated [206].

9.3.5.1. BCG and ICL

The brightest cluster galaxies (BCGs), residing in the center of galaxy clusters, are the most massive and luminous galaxies. Traditionally, they are the most difficult

galaxies to be properly reproduced in simulations, as they suffer dramatically from the so-called “over-cooling” problem when the feedback description in the simulations is incomplete [208–210]. In addition, they encounter many interactions with satellite galaxies and significantly grow through mergers. Such destructive events also lead to the growth of a diffuse intracluster light (ICL) or diffuse stellar light (DSL), which may contain a significant fraction of the total stellar component in clusters (see [211] and references therein). The velocities of the stars in a cD galaxy and ICL have dynamically well-distinct kinematic distributions, which can be characterized by two Maxwellian distributions. While the velocity dispersion of the stars in the cD galaxy represents the central mass of the stars, the velocity dispersion of the ICL is much larger and comparable to that of the DM halo [212–214]. Early simulations found that the density distributions can be described by a superposition of two extended components [208]. However, more recent simulations find that in many cases (ignoring the very central part), it can be described by a single, radial profile (in good agreement with observations) and only in rare cases need to be described by the sum of two extended components with different radial shapes. Interestingly, the three-dimensional distribution of this outer stellar halo seems to be described universally by a so-called Einasto profile over a wide range of halo masses [215]. Simulations which do not suffer from the overcooling problem also reproduce the observed mass–radius relation for such massive, early-type galaxies [209, 216].

9.3.5.2. *Cluster galaxies*

Although reproducing the exact stellar mass function, especially for the most massive galaxies, is still quite challenging for hydrodynamical simulations due to uncertainties in our understanding of stellar and AGN feedback processes, the strong environmental imprint onto cluster members is already present in even moderately resolved simulations and independent of the details of the implemented feedback [217]. For example, the removal of gas from cluster member galaxies and the subsequent turn off of star formation are naturally captured by hydrodynamical simulations, while such processes are challenging to capture properly in semianalytic modeling [218]. However, reproducing the observed radial distribution of member galaxies, especially in the central region of galaxy clusters, is still one of the challenges of modern simulations, as high numerical resolution is required in order to resolve the stellar distributions within galaxies. A similar problem is also reflected in the still uncertain origin of the discrepancies between simulations and observations in the evolution of the orbital properties of cluster members (see [219] and references therein). Besides these issues on the internal properties of cluster galaxies on small scales, hydrodynamical simulations are capable of reproducing the differential clustering power of galaxies [220], where interactions with the cluster environment is one of the main drivers.

9.4. Beyond prevalently treated processes

Additional components in the ICM, such as cosmic rays (CR) and magnetic field, could provide additional nonthermal pressure support in galaxy clusters. However, these nonthermal components of the ICM can be detected only indirectly, making their interpretation a challenging task. For example, synchrotron radiation reflects the complex combination of the integrated magnetic field structure and cosmic ray electron (CRe) distribution, while Faraday Rotation measurements provide information about the strength and structure of magnetic field. CR protons (CRp) should also reveal their presence by producing γ -ray photons through hadronic interactions with thermal ions in the ICM. Transport processes, such as thermal conduction, can also affect the thermodynamic properties of the ICM, but the efficiency of the transport processes depends on the still poorly understood nature of magnetic field. Additional plasma physics effects, such as electron–ion equilibration or sedimentation of heavier elements, can further complicate the interpretation of the ICM properties inferred by astronomical observations. In this section, we will discuss our current understanding of these nonthermal processes in galaxy clusters.

9.4.1. *Magnetic fields in clusters*

Magnetic fields on large scales are observed within galaxies, along their outflows (see [221] for a recent review) and even all galaxy clusters are known to host magnetic fields with strengths up to several μG [222], which influences the dynamics of the hot plasma. The structure and the amplitude of the cluster magnetic fields guide the propagation of charged particles and contribute to the equation of motion via the Lorentz force, giving effectively a nonthermal pressure component.

The magnetic field can be inferred via synchrotron emission, where the intensity gives a measure of the magnetic field strength and the polarization data yield its orientation. Additionally, Faraday Rotation measurements reveal information about the integrated magnetic field component along the line of sight (see [223] for a recent review and references therein).

Within the ICM, the inferred magnetic fields from synchrotron emission range from 0.1 to 0.5 μG on scales up to 1 Mpc. Faraday Rotation measurements provide consistent result and also reveal strong magnetic fields up to 30 μG inside cooling cluster cores, especially around AGNs [224]. The magnetic field lines are assumed to be highly tangled and twisted on small scales, as inferred from the structures within Faraday Rotation measurements observed against radio lobes within galaxy clusters [225, 226]. Galaxy clusters with multiple radio galaxies can also constrain the shape of the radial magnetic field profile [173].

9.4.1.1. *Simulating magnetic fields in clusters*

Magnetohydrodynamic (MHD) simulation is a method of choice for studying the evolution of magnetic fields in galaxy clusters [228–236]. These ideal MHD

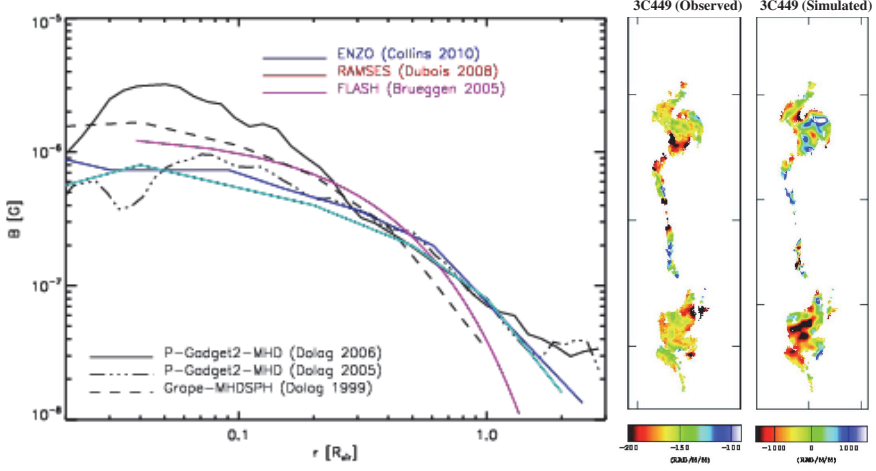


Fig. 9.13. *Left panel:* Normalized magnetic field profiles in galaxy clusters, predicted by several nonradiative simulations. *Right panel:* Comparison of the predicted RM map from numerical simulations with the observed map of 3C449. Figure taken from Ref. [227]

simulations suggest that the hierarchical structure formation process through accretion and mergers can generate turbulent gas motions, which in turn amplify weak magnetic field to the observed μG level through the turbulent amplification process [237].

Figure 9.13 shows the comparison of the radial magnetic field profiles of galaxy clusters from various simulations. The resulting magnetic fields show a significant radial decline similar to the gas density profile [238] (see the left panel of Fig. 9.13). The structure of the magnetic field is driven primarily by the internal dynamics of merging galaxy clusters and is fairly insensitive to the properties of the seed magnetic fields [239]. The turbulent nature of the amplification process also leaves an imprint on the expected pattern of rotation measure of radio lobes within clusters [227, 240] (see the right panel of Fig. 9.13).

However, the exact shape of the predicted magnetic field profile in these simulations depends on the amount of magnetic dissipation (originating from either artificial induced by the numerical implementation or originating from the underlying spatial resolution [227, 236] or physically motivated, macroscopic magnetic resistivity [241]) within the ICM as well as galaxy formation processes, such as gas cooling, star-formation and stellar or AGN feedback. For example, the baryon compression process induced by gas cooling can amplify the magnetic field through the turbulent dynamo on small scales (e.g., cool cores in the center of galaxy clusters or cluster galaxies), while feedback processes can further contribute to the amplification of magnetic fields by injecting more turbulence within the ICM [232, 242, 243]. Despite these uncertainties, the magnetic fields with the observed level of a few μG contribute up to a few percent of the thermal energy density of the ICM.

9.4.1.2. *Origin of magnetic fields in clusters*

The origin of magnetic fields on scales of galaxies and galaxy clusters is still under debate. A variety of mechanisms have been proposed, including primordial fields (see [245] for a review), battery fields [246, 247] and various classes of astrophysical objects which contribute with their ejecta [248–250].

The generation of magnetic fields by the so-called Bierman battery effect has been pioneered in cosmological simulations by [246, 247]. However, such simulation must assume successive amplification of the fields through small-scale dynamo in order to lift weak battery fields to the observed amplitude before they get re-structured by the cluster formation process as described before.

Models which invoke seed fields from AGN outflows [251] or galactic winds [244], on the other hand, are capable of amplifying the seeds fields to the observed strength by the structure formation process without additional assumptions. Although different models result in similar magnetic fields in clusters, different seeding mechanisms result in dramatically different magnetic fields in large-scale filament or voids [244] (see also Fig. 9.14).

Recently, there has been attempts to couple the seeding of magnetic field directly to the star-formation process. In these simulations, the rate of SN explosions

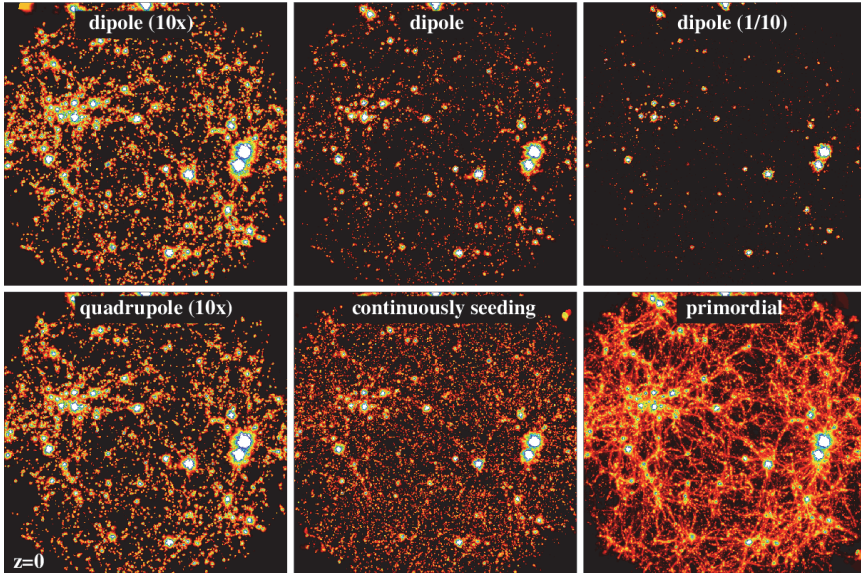


Fig. 9.14. Visualization of the magnetic field strength in a simulation box at redshift $z = 0$ for different models of galactic outflow seeding. Upper panels show the effect of varying the amplitude of seeded galactic magnetic field by a factor of ± 10 around the fiducial model shown in the center. Left columns show the difference between a dipole and a quadrupole galactic field. Lower-middle panel shows the effect of including multiple seeding events, while the lower-right panel shows the results for a primordial, space-filling magnetic seed field. Figure taken from Ref. [244].

is self-consistently calculated from the local star-formation rate [252, 253], and small-scale seed magnetic fields with typical dimensions and magnetic field amplitudes as found in canonical SN remnants are injected. Such simulations have been generally capable of reproducing the observed magnetic field strength in galactic halos [70], galactic disc [253], and galaxy clusters [254].

The understanding of the structure and evolution of magnetic fields within the ICM is important, as their detailed properties (e.g., strength and shape) ultimately control transport processes (such as thermal conduction and viscosity) in the ICM.

9.4.2. *Thermal conduction*

Thermal conduction has been frequently discussed as a possible heating source to balance cooling losses in the central region of galaxy clusters, where the cooling time is significantly shorter than the cluster lifetime.

9.4.2.1. *Isotropic conduction*

For an unmagnetized plasma, a conduction heat flux resulting from a temperature gradient is given by [257]

$$\vec{Q} = -\kappa \vec{\nabla} T, \quad (9.12)$$

where the effective conductivity κ is given by [258]

$$\kappa = 4.6 \times 10^{13} \left(\frac{T_e}{10^8 K} \right)^{5/2} \frac{40}{\ln \Lambda} \frac{\text{erg}}{\text{s cm K}}, \quad (9.13)$$

where n_e is the number density, T_e the temperature, m_e the mass of electrons, and the Coulomb logarithm is given by, $\ln \Lambda \approx 37.8$.

Because of the strong dependence of conductivity on the electron temperature, thermal conduction plays the most important role in the central regions of massive galaxy clusters, where the ambient plasma temperature reaches up to about $10^8 K$ along with the strong temperature gradient in the cool core region. Note that light electrons are considerably more efficient heat carriers than heavier ions.

For a realistic case of the magnetized ICM, the influence of the magnetic field on thermal conduction must be taken into account [259–266]. For a simple case of a tangled magnetic field, this is taken into account by introducing a suppression factor of $1/3$ of the Spitzer value [267]. However, although the isotropic conduction with $1/3$ of the Spitzer value can significantly change the temperature profile in hot galaxy clusters, it fails to resolve the overcooling problem in simulations [254, 268]. In addition, it leads to significantly reduced temperature structures in the ICM (which can be seen in the examples shown in Fig. 9.15) to the point that it may be inconsistent with recent observations (see the left panel of Fig. 9.16).

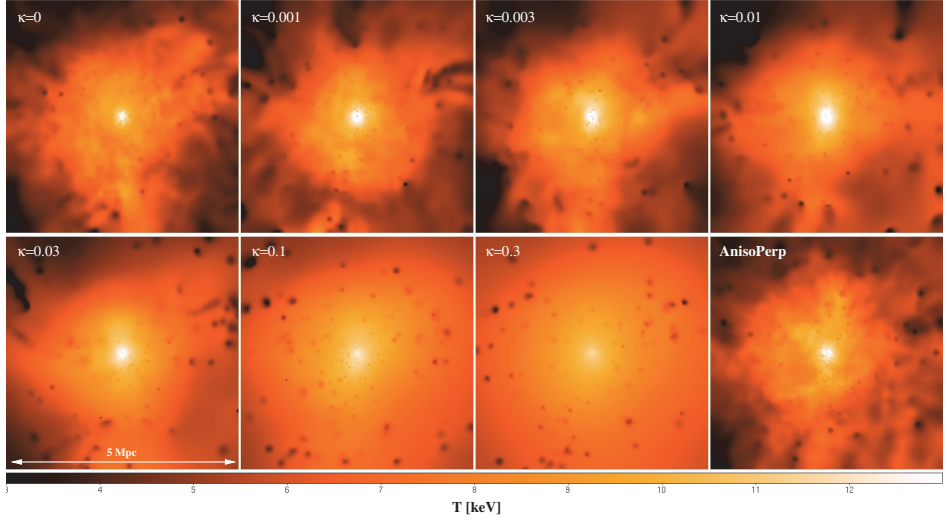


Fig. 9.15. The mass weighted temperature maps ($5 \text{ Mpc} \times 5 \text{ Mpc}$) of the relaxed, massive cluster at $z = 0$ are shown. The upper left panel shows the simulation without any thermal conduction. The other maps (from upper left top lower right) show the sequence for isotropic thermal conduction when changing the suppression factor as indicated in the maps. The lower right panel shows the run with anisotropic thermal conduction where the perpendicular term is evaluated proportional to the magnetic field strength. Figure taken from Ref. [254].

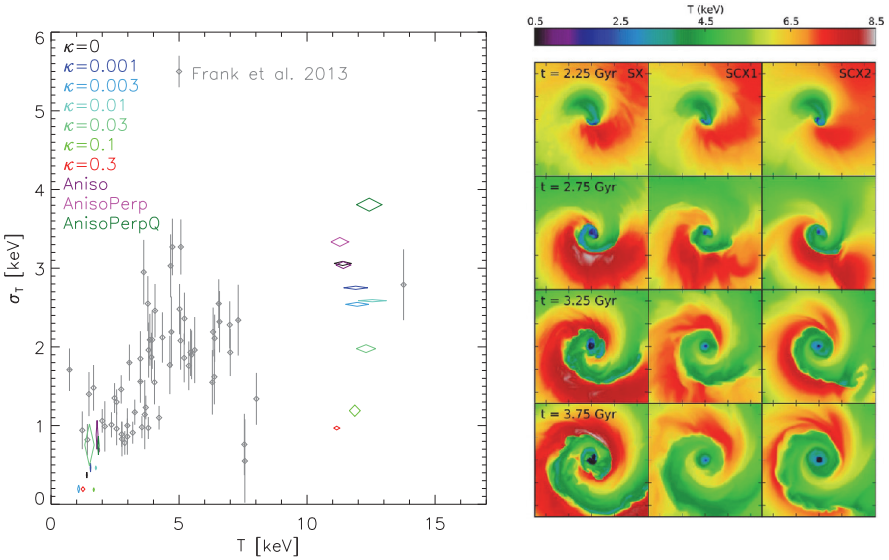


Fig. 9.16. *Left panel:* Comparison of the temperature fluctuations within R_{2500} as inferred from observations by [255] with the one predicted for a simulated cluster (see Fig. 9.15) with different treatment of the thermal conduction (as labeled). Taken from [254]. *Right panel:* Temperature slices through the centre of a sloshing core simulation at different times, showing a 500 kpc region. Left column is without conduction. Central and right columns are performed with anisotropic conduction with varying initial magnetic field configurations. Figure taken from Ref. [256].

Observational evidence in galaxy clusters of strongly suppressed heat transport is found in a so-called cold front, a contact discontinuity characterized by sharp density and temperature gradients, but no pressure gradient. This phenomenon demonstrates the insulation of gas with respect to conduction most probably through magnetic fields (see [269] for a review and references therein).

9.4.2.2. *Anisotropic conduction*

In the presence of magnetic fields, electrons can only move on spiral trajectories around the field lines, leading to anisotropic conduction along the field line. The conductive heat flux in the magnetized medium is then given by

$$\vec{Q} = \underbrace{-\kappa_{\parallel} \vec{\nabla}_{\parallel} T}_{\text{collisional}} - \underbrace{\kappa_{\perp} \vec{\nabla}_{\perp} T}_{\text{"suppressed"}} - \underbrace{\kappa_{\Lambda} \vec{B}_{\text{norm}} \times \vec{\nabla} T}_{\text{noncollisional, vanish for large } \vec{B}}, \quad (9.14)$$

with the parallel (to $\vec{B}$) term $\kappa_{\parallel}$, the perpendicular (to $\vec{B}$) term $\kappa_{\perp}$ and the hall term κ_{Λ} [270]. It is generally nontrivial to write down how $\kappa_{\parallel}$, $\kappa_{\perp}$ and κ_{Λ} should generally be related to κ and how it should scale with the magnetic field strength, especially in the limit of the discretization used and the scales represented in the simulation. To date, there have been a number of hydrodynamic simulations with anisotropic conduction [254, 256, 271–282]. Note that some of these simulations include the $\kappa_{\perp}$ term [254, 256, 271, 273, 277, 279], while none includes the Hall term explicitly (although the Hall term vanishes in a certain discretization, such as the one used in [254]).

The effect of anisotropic conduction is that it, in principal, can drive the magnetothermal instability (MTI) [148, 149] in the cluster outskirts and the HBI [153] in the cluster center. However, cosmological simulations of galaxy clusters demonstrated that gas motions generated by these instabilities do not play a significant role because turbulent motions tend to reset the (radial) orientation of the magnetic field that the MTI tries to establish [283]. In cluster cores, the gas motions generated by HBI even in their most optimistic scenario are less than 10 km/s, which is orders of magnitude less than gas motions generated by cosmic accretion or SNe/AGN feedback [284], and the effects of HBI may be further suppressed in combination with anisotropic viscosity [285]. Therefore, it remains unclear if these plasma instabilities have a notable impact onto the structure and evolution of the ICM.

While thermal conduction is inefficient in suppressing gas cooling in cluster cores, anisotropic conduction can modify the temperature structure of the ICM due to the coupling of the suppression factors to the local dynamical state of the cluster [254, 282]. Effects of anisotropic conduction on the properties of cold fronts generated by sloshing gas motions have also been investigated [256] (see the right panel of Fig. 9.16). In both cases, contrary to the case of isotropic heat conduction,

anisotropic conduction produces a reasonable amount of temperature fluctuations compared to observations and still allows transport of heat locally (Fig. 9.17).

9.4.3. *Cosmic rays*

There are several possible contributors to the population of CR in the ICM, including AGN and stellar activities in cluster galaxies and shock waves generated by cluster mergers (see [286, 287] for reviews). There are two main components of CR in galaxy clusters. The light and fast-cooling CRe are seen in gigantic, merger-driven shock waves, where turbulent motions reaccelerate mildly superthermal electrons or they originate as secondary products of hadronic interactions of CRp with thermal ions in the ICM. Being a light component, CRe do not significantly contribute to the pressure of the ICM, but show up as synchrotron radiation in the presence of magnetic fields. The heavier and slow-cooling CRp, on the other hand, keep a fossil record of various processes, such as star formation, AGN activities and accretion shocks. CRp might also play a role in regulating star formation through their dynamical imprint on the interstellar medium (ISM), driving energetic outflows from galaxies, and potentially contributing to the ICM pressure.

9.4.3.1. *Cosmic ray protons*

Due to their very long cooling time ($> 10^{10}$ years), CRp are expected to accumulate within galaxy clusters over their lifetime and therefore could contribute significantly to the ICM pressure. Self-consistent simulations of CR in galaxy clusters follow the evolution of CRe and CRp injected by cosmological structure formation shocks [289, 290] or the combination of shocks and contribution from supernovae [291]. However, the dynamical role of CR in galaxy clusters is not very well understood yet. Simulations using different model assumptions predict quite different relative pressure contained in CRp within galaxy clusters. Moreover, these simulations indicate that the relative importance of CRp in galaxy clusters also depends on other nonthermal processes, such as radiative losses and feedback from star formation [18].

The CRp population within galaxy clusters is also expected to interact hadronically with thermal ions in the ICM [292] and thereby produce pions. The charged pions decay into secondary electrons (and neutrinos), and the neutral pions decay into γ -rays photons. Despite many attempts to observe γ -ray emission from galaxy clusters, no such detection has been obtained so far (see [288] and references therein). The lack of detection of γ -ray emissions by Fermi γ -ray space telescope observations of galaxy clusters indicate that the energy budget of CRp in galaxy clusters is limited to the percent level of the thermal energy in nearby, rich clusters [293–295].

9.4.3.2. *Cosmic ray electrons*

Nonthermal emission is observed in the radio band from galaxy clusters (see [223] for a recent review and references therein), most spectacularly in the form of giant

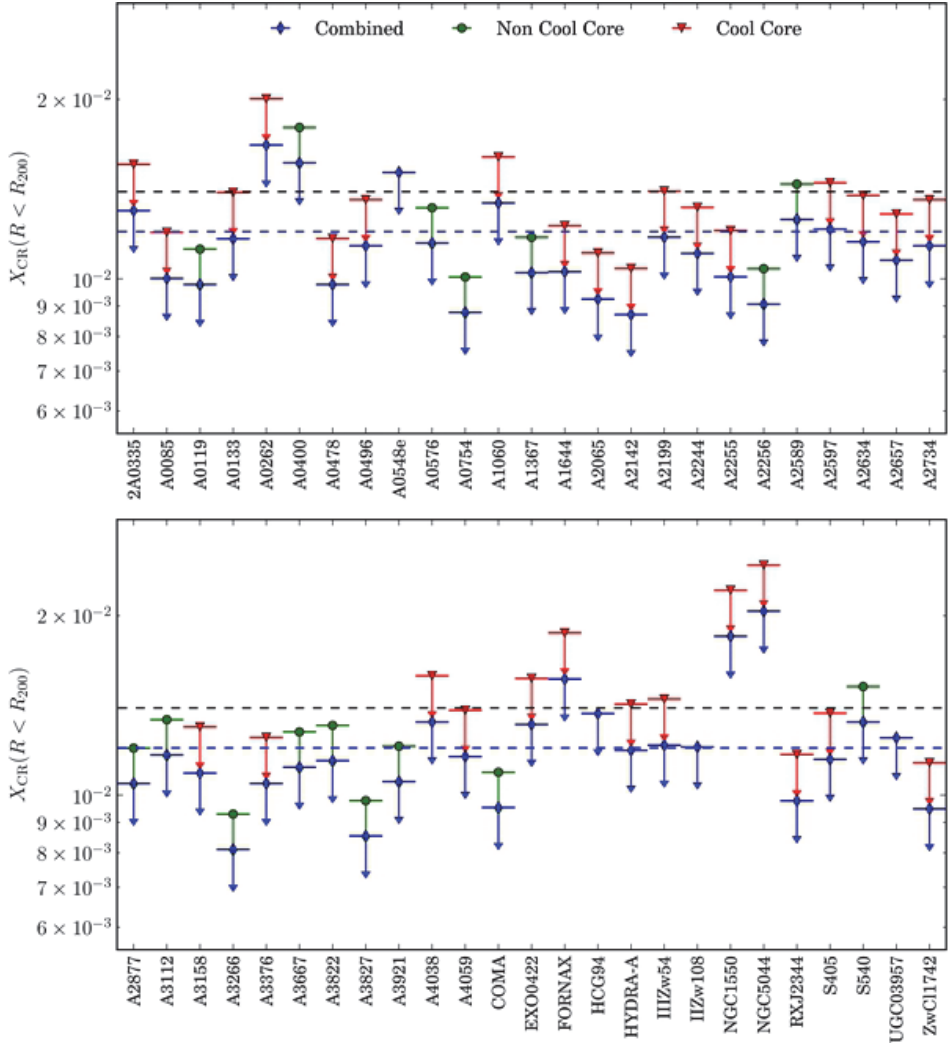


Fig. 9.17. 95% upper limits on cosmic ray pressure for 50 nearby galaxy clusters obtained from nondetection of γ -ray emission by Fermi LAT. Figure taken from Ref. [288].

radio halos. The origin of the underlying synchrotron bright CRe lightening up in the cluster magnetic field is still unclear, although the commonly discussed mechanisms include (1) reacceleration by merger-driven turbulence [298–302] and (2) the *in situ* production of CRe by proton–proton collisions [292, 303–305], or (3) a combination of the two mechanisms [306, 307].

To date, pure secondary models appear disfavored by radio spectra of some halos [308–312]. In addition, γ -rays are unavoidably produced by the same decay chain in these models, but clusters have not yet been observed in γ -ray band to date, as discussed before. This leaves hadronic models assailable. Today, the reacceleration

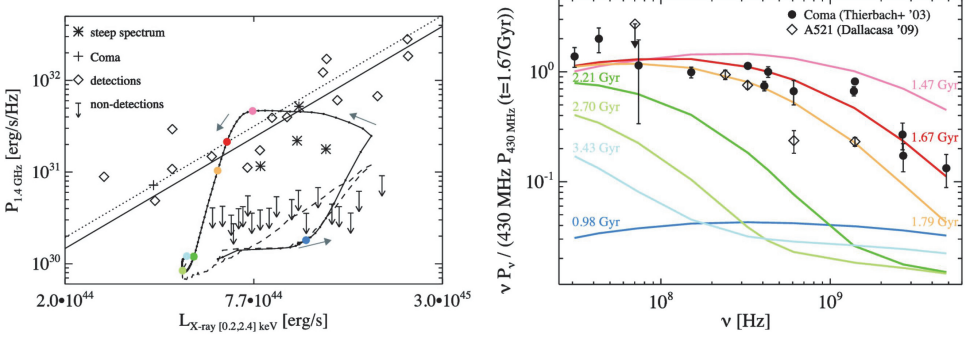


Fig. 9.18. *Left panel:* Evolution of a galaxy cluster merger in X-rays and radio synchrotron emission as the black line. The dots on the lines are placed at an interval of 25 Myr. The colored dots correspond to the times shown in the right panel. Overplotted are observed radio halos and upper limits [296]. *Right panel:* Radio synchrotron spectrum from a cluster merger simulation at different times. The observed spectrum of Coma and A521 are indicated with solid-black circles and open-diamond, respectively. Figure taken from Ref. [297].

by merger-driven turbulence is considered to be the most likely explanation for the appearance of giant radio halos, although the underlying theory is quite complex and not yet fully understood ([313] for a recent review).

Recently, there have also been some attempts to simulate the spectral evolution of the CRe distribution, either directly for the SPH particles [297] or by using tracer particles in Eulerian simulations [314, 315]. This is a numerically challenging problem, and only a small number of such direct simulations exist to date, mostly done in post-processing. However, such models have been successful in reproducing some of the key observable properties of giant radio halo [297] (see the left panel of Fig. 9.18). So far, the simulations have been successful in reproducing the shape of the spectrum as observed in radio halos (see the right panel of Fig. 9.18). This spectral shape is driven by the fact that the energy-dependent cooling time of the CRe distribution leads to a curvature in the CRe distribution, which manifests in a curvature in the radio spectrum [308]. These simulations also show a proper evolution of the radio halo brightness after the merger event. However, due to the decaying turbulence, the fast cooling CRe in these simulations cannot be refreshed, which causes the radio halo to fade quickly and hence produce galaxy clusters without radio emission, as frequently observed.

The second class of large-scale radio emission in galaxy clusters are the so-called radio relics [223, 316, 317], which in contrast to radio halos are polarized and thought to be produced by shock waves in merging galaxy clusters. Cluster merger shocks accelerate relativistic electrons, which subsequently interact with the magnetic field and emit synchrotron radiation. The main features of the extended peripheral radio emission (so-called radio relics) observed in A 3667 have been reproduced by combining the single merger simulations with a model for the *in situ* reacceleration of the relativistic particles [318]. The distribution of the Mach numbers of the shocks

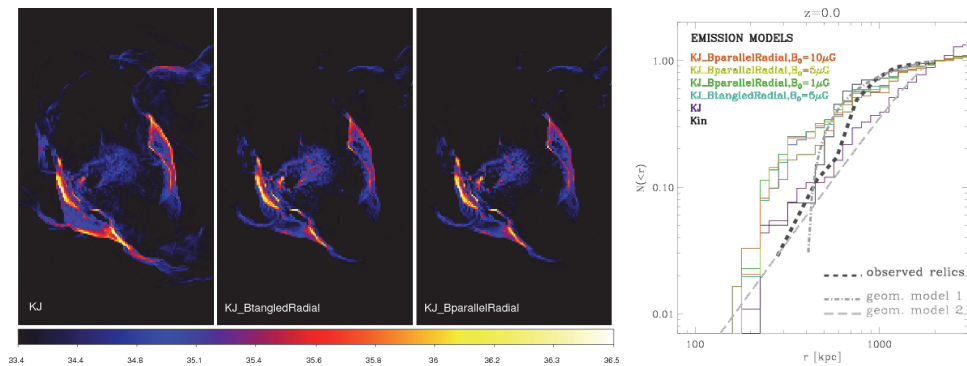


Fig. 9.19. *Left panels:* Emitted “radio” power from simulated relics for the same galaxy cluster at $z = 0$ and for three emission models. The side of each image is 10 Mpc/h. *Right panel:* Cumulative distributions of simulated radio *gischt* relic for different emission models. The dashed dark gray line is for observed radio relics. Figure taken from Ref. [314].

within the cosmological structures and their role in producing radio relics in galaxy clusters have also been investigated either by semianalytical modeling (see [319, 320] and references therein) or by cosmological simulations based on various numerical implementations — either as post-processing of the simulations or directly on the fly [290, 315, 321–326]. The appearance of simulated radio relics can be compared with observations, although such comparisons are still limited as the obtained radio emission depends on various assumptions on the acceleration efficiencies and the magnetic field. Figure 9.19 shows an early attempt for such a comparison by [314], although the details (such as the efficiency of the diffusive shock acceleration) still remain unclear [327]. There is also a possibility that the shocks do not directly accelerate electrons from the thermal pool but rather re-energize (by compression) or reaccelerate fossil radio plasma escaped from radio galaxies [328]. Interestingly, recent observations report some evidence of such a process in the merging galaxy clusters Abell 3411–3412 [329].

9.4.4. *Electron–ion equilibration in cluster outskirts*

X-ray and SZ measurements of hot gas in galaxy clusters are often interpreted under a number of simplifying assumptions on the poorly understood physics of the intracluster plasma. These assumptions, if not understood and accounted for, could be significant sources of systematic errors in cosmological measurements. For example, observational probes of this gas are generally sensitive only to the electron component of the plasma. Typically, theoretical studies assume that the electrons are in thermal equilibrium with the surrounding ions; i.e., $T_e = T_i$. However, this is not a good approximation in the low-density outskirts of galaxy clusters due to the extended timescale for electrons to reach equilibrium via Coulomb collisions [331–334]. When an electron–ion plasma passes through a shock, most of the

kinetic energy goes into heating the heavier ions, causing $T_i \gg T_e$.³ After the shock, electrons and ions slowly equilibrate via Coulomb interactions, each converging to the mean gas temperature, $T_{\text{gas}} = (n_e T_e + n_i T_i) / (n_e + n_i)$, over a typical electron–ion equilibration timescale, t_{ei} . The evolution of the electron temperature is given by

$$\frac{dT_e}{dt} = \frac{T_i - T_e}{t_{ei}} - (\gamma - 1)T_e(\nabla \cdot \mathbf{v}), \quad (9.15)$$

where the second term accounts for adiabatic compression heating and cooling. The timescale for equipartition between two charged species is given by [335],

$$t_{eq} = \frac{3m_1 m_2}{8(2\pi)^{1/2} n_2 Z_1^2 Z_2^2 e^4 \ln \Lambda} \left(\frac{kT_1}{m_1} + \frac{kT_2}{m_2} \right)^{3/2}, \quad (9.16)$$

where m , T , and Z are the mass, temperature, and charge of each species, respectively, n is the number density, and $\ln \Lambda \approx 40$ is the Coulomb logarithm. For the fully ionized ICM, including contributions from both protons and He^{++} , the timescale for equilibration is

$$t_{ei} \approx 6.3 \times 10^8 \text{yr} \frac{(T_e/10^7 \text{K})^{3/2}}{(n_i/10^{-5} \text{cm}^{-3})(\ln \Lambda/40)}. \quad (9.17)$$

Note that this timescale can be comparable to the Hubble time in regions with $T \sim 10^7$ K and overdensities 10–100 with respect to the cosmic mean (Fig. 9.20).

In the outskirts of galaxy clusters, the collision rate of electrons and protons becomes longer than the age of the universe. The lower electron temperature in the cluster outskirts leads to a significant underestimate of the gas pressure when derived through the SZ effect. This deviation is larger in more massive and less relaxed systems, ranging from 5% in relaxed clusters to 30% for clusters undergoing major mergers. The presence of nonequilibrium electrons leads to significant suppression of the SZ effect signal at large cluster-centric radius. The suppression of the electron pressure also leads to an underestimation of the hydrostatic mass. Merger-driven, internal shocks may also generate significant populations of nonequilibrium electrons in the cluster core, leading to a 5% bias on the integrated SZ mass proxy during cluster mergers [330].

9.4.5. Helium sedimentation

Another commonly adopted assumptions in X-ray cluster analyses is the uniformity of the helium-to-hydrogen (He-to-H) abundance ratio with nearly primordial

³Note that we divide the plasma into two components, electrons and ions, which are assumed to be individually in local thermodynamic equilibrium with separate Maxwellian velocity distributions defined by temperatures T_e and T_i , respectively. The separation into only two species, electrons and ions, each in separate equilibrium is reasonable, since the self-equilibration timescales for each species, t_{ii} and t_{ee} , are considerably shorter than the electron–ion equilibration timescale, t_{ei} [331, 335]. ($t_{ei} \sim (m_i/m_e)^{1/2} t_{ii} \sim (m_i/m_e)^{1/2} t_{ee}$.)

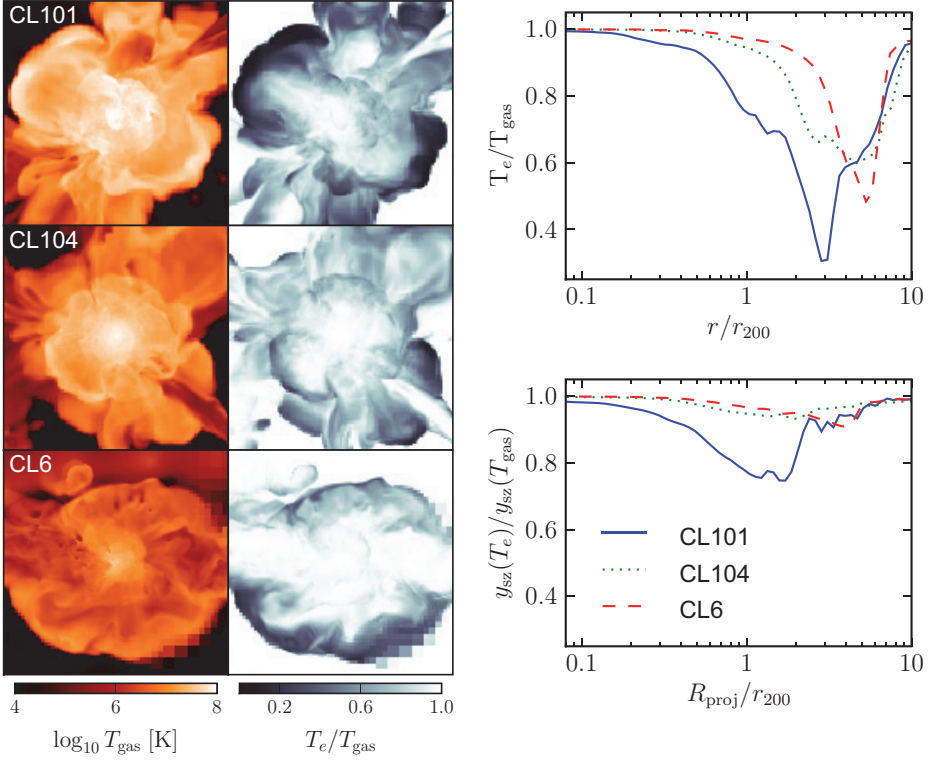


Fig. 9.20. *Left panels:* The distribution of the mean gas temperature (T_{gas} , left column) and the ratio of electron and mean gas temperatures (T_e/T_{gas} , right column) for three simulated clusters at $z = 0$. The projected mass-weighted gas temperature in $1h^{-1}$ Mpc slices centered on each cluster and $12h^{-1}$ Mpc on a side. *Right panels:* Profiles of ICM electron temperature relative to the mean ICM gas temperature for each cluster at $z = 0$: 3D electron temperature profiles plotted averaged in spherical shells and scaled to r_{200} (top panel) and 2D mass-weighted electron temperature profiles averaged in cylindrical annuli projected $60h^{-1}$ Mpc through the simulation volume (bottom panel). This quantity is equivalent to the bias in the observed SZ flux in each annulus with respect to the flux one would observe if the electron temperature, T_e , were equal to the mean gas temperature, T_{gas} . Figure taken from Ref. [330].

composition in X-ray emitting ICM. At present, there is no observational test of this assumption, since both H and He in the ICM are fully ionized, which makes it difficult to measure their abundances using traditional spectroscopic techniques.

Theoretically, it has long been suggested that heavier He nuclei slowly settle in the potential well of galaxy clusters and cause a concentration of He toward their center [337–342], where particle diffusion in clusters is characterized by the Burgers equations of a multicomponent fluid [343]. Observationally, the ICM properties derived from X-ray observations depend on the assumed value and profile of the H-to-He abundance ratio, since the observed X-ray surface brightness arises primarily

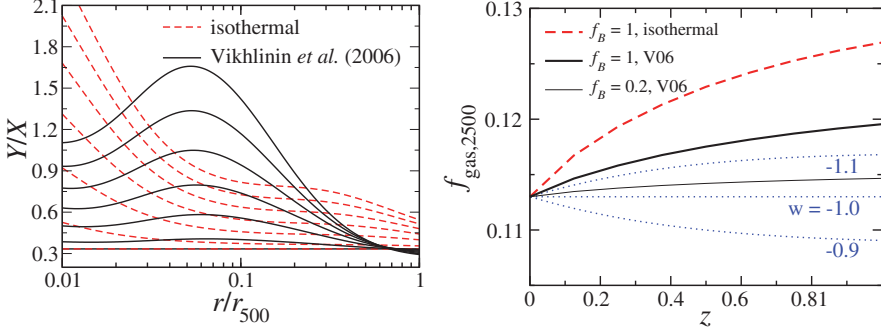


Fig. 9.21. *Left panel:* The radial profile of helium-to-hydrogen mass fraction (Y/X) in a $T_X = 10$ keV static cluster with $f_B = 1$. Lines indicate two types of ICM temperature profiles: (1) the simple isothermal profile, and (2) observed temperature profile for a cluster with 0, 1, 3, 5, 7, 9, and 11 Gyr (from bottom to the top), respectively. *Right panel:* Evolution of cluster gas mass fraction enclosed within R_{2500} as a function of redshift of a 10 keV cluster with a realistic MAH. Lines indicate the isothermal model with $f_B = 1$ (dashed line), V06 model with $f_B = 1$ (thick-solid line), and $f_B = 0.2$ (thin-solid line). Dotted lines indicate the evolution in f_{gas} caused by changes in the dark energy equation of state w by 10% relative to the fiducial Λ CDM cosmological model with no sedimentation indicated by a straight dotted line. Figure taken from Ref. [336].

from bremsstrahlung emission of electrons scattering off of protons and He nuclei,

$$S_X \propto \int dl (n_e n_p \Lambda_{ep} + n_e n_{\text{He}} \Lambda_{e\text{He}}) \quad (9.18)$$

$$\propto n_p^2 (1 + 2x)(1 + 4x) \Lambda_{ep}, \quad (9.19)$$

where $x \equiv n_{\text{He}}/n_p$ is the He-to-H abundance ratio and Λ_{ei} is the band-limited cooling function resulted from free-free emission of electrons scattering off ion species i , which is proportional to Z_i^2 . For fully ionized H-He plasma, the number density of electron and protons are given by $n_e = n_p + 2n_{\text{He}} = n_p(1 + 2x)$.

In the era of precision cosmology, this could be a source of significant systematic uncertainties in X-ray measurements of galaxy clusters and cosmological parameter derived from these measurements [269, 336]. For example, Fig. 9.21 shows the effect of He sedimentation is degenerate with the effect of the equation of state of dark energy, w . These biases introduce an apparent evolution in the observed gas mass fractions of X-ray luminous, dynamically relaxed clusters and hence biases in observational constraints on the dark energy equation of state parameter, w , derived from the cluster distance-redshift relation. The Hubble parameter derived from the combination of X-ray and SZE measurements is affected by the He sedimentation process as well. Future measurements aiming to constrain w or H_0 to better than 10% may need to take into account the effect of He sedimentation. For cosmological measurements, one way to minimize these biases is to extend the X-ray measurements to a radius well beyond R_{2500} . At the same time, the evolution of cluster gas mass fraction in the inner regions of clusters should provide unique observational diagnostics of the He sedimentation process in clusters.

9.5. Outstanding challenges and future prospects

Recent years have witnessed the emergence of galaxy clusters as powerful laboratories for astrophysics and cosmology. Being the largest and most magnificent structures in the Universe, clusters of galaxies serve as excellent tracers of the growth of cosmic structures. The current generation of X-ray and SZ cluster surveys have provided independent confirmation of the cosmic acceleration and significantly tighten constraints on the nature of mysterious dark energy and DM as well as new insights into how massive galaxies and BHs form and grow in the Universe.

For example, cluster surveys based on the SZ effect has reported tension in cosmological inferences from CMB and galaxy clusters, suggesting either that we discovered new physics (e.g., the mass of neutrinos) or an unexpectedly large bias in the mass estimates of galaxy clusters. In order to resolve this so-called “Planck CMB–Cluster tension”, multiwavelength observational campaigns with *Chandra* and XMM-*Newton* X-ray space observatories as well as gravitational lensing measurements in optical are underway to follow-up over several hundred SZ-selected clusters by the South Pole Telescope (SPT), Atacama Cosmology Telescope (ACT), and Planck space mission.

The next decade promises to be especially exciting as the next generation of multiwavelength cluster surveys are expected to discover over 100,000 galaxy clusters: Spectrum-RG/eROSITA (German-Russian: scheduled to launch in 2018), Advanced ACTPol, SPT-3D, and other CMB-StageIV experiments (in US) in microwave, Dark Energy Survey (DES: US), Dark Energy Spectroscopic Instrument (DESI: US), Euclid (international project led by EU), Large Synoptic Survey Telescope (LSST: international project led by US), Subaru HSC (Japanese-US), Wide-Field Infrared Survey Telescope (WFIRST: international project led by US) in optical. However, the statistical power of future cluster surveys can be exploited for cosmology if and only if we can improve our understanding of cluster astrophysics and reduce astrophysical uncertainties in cluster mass estimates. Significant advances in computational modeling of galaxy clusters will be critical for interpreting and exploiting large datasets from upcoming multiwavelength cluster surveys.

Numerical simulation is the method of choice for studying the formation and evolution of galaxy clusters. Remarkably, modern hydrodynamical cosmological simulations are capable of following the dynamics of DM, stars, and gas in their full complexity during the hierarchical build-up of structures. These simulations also suggest that astrophysical uncertainties in the cluster mass estimates originate from turbulent gas motions, inhomogeneities in the gas density and temperature structures, energy injection from AGN residing in the cluster center, and plasma physics, where the bracket indicates systematic uncertainty associated with each astrophysical process. Achieving the requisite accuracy in the cluster estimate thus requires improved understanding of plasma physics on nanoscales to gravitational dynamics on cosmological scales.

To address this problem, advances in theoretical and computational modeling of galaxy clusters are especially important, and they will hold the key for realizing the statistical power of large datasets from upcoming large cluster surveys. This poses a challenging multiscale physics problem involving the large-scale structure formation to the microphysics of galaxy clusters. Specifically, future advances in computational modeling of galaxy clusters should focus on (1) advancing our understanding of the physics of galaxy cluster formation, (2) developing novel, low-scatter mass proxies for upcoming multiwavelength cluster surveys, and (3) ultimately reducing astrophysical uncertainties in the cluster mass estimates of order a few percent, which would be a dramatic improvement from the present 10–30% uncertainty reported in the literature. One promising avenue lies in focusing on the outskirts of galaxy clusters, which are expected to be much less susceptible to the poorly understood baryon physics (such as gas cooling, star formation, and energy feedback from stars and AGN) than the well-studied but more complex cluster core regions. It is a particularly important contributor to the SZ signal. This makes the outskirts of galaxy clusters ideal locations for making robust measurements of galaxy cluster masses.

Future work should thus focus on bringing together expertise and resources to develop a variety of (both cosmological and idealized) simulation codes to investigate and constrain a variety of astrophysical phenomena (such as turbulence, magnetic field, cosmic rays, plasma physics, and energy injection from stars and AGN) on a variety of observables (such as hot X-ray emitting ICM and cluster galaxies) and scales (from cores to outskirts of galaxy clusters) through detailed comparisons of numerical simulations and multiwavelength observations (see Video 8, page xiii).

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Preface

This volume of *Encyclopedia of Cosmology* is devoted to the explanation of theoretical and observational aspects of dark energy. The book is mainly for PhD students and researchers who would like to learn the fundamentals of dark energy. I begin here to explain the basics of general relativity and then proceed to the cosmic expansion history from primordial eras to today. People who do not have the knowledge of general relativity can gain its necessary information from this volume and also access modern theoretical cosmology.

The discovery of cosmic acceleration in 1998 opened up a new research field in cosmology. Before this discovery, it was believed that the expansion of the Universe today is decelerating. However, the observations of distant supernovae type Ia (SN Ia) showed that they looked fainter than the expected decelerating Universe. The observational data of SN Ia suggested that the Universe today is accelerating.

Dark energy is an unknown form of energy introduced to account for the late-time cosmic acceleration. The simplest candidate for dark energy is a cosmological constant, whose energy density stays constant even on an expanding background. Assuming that the origin of dark energy is the cosmological constant, Riess *et al.* and Perlmutter *et al.* independently showed that about 70% of the total energy density of the today's Universe consists of the cosmological constant.

The cosmological constant was first introduced by Einstein in 1916 to realize a static Universe. In the Einstein's static Universe, a negative pressure induced by the cosmological constant balances with the gravitational attraction. After the discovery of cosmic expansion by Hubble in 1929, Einstein regretted the fact of introducing the cosmological constant. In 1998, however, the cosmological constant was revived as a source for dark energy. In modern context, the negative pressure of the cosmological constant overwhelms the gravitational attraction for realizing the acceleration of the Universe.

After 1998, other observational data such as those from Cosmic Microwave Background (CMB), Baryon Acoustic Oscillations (BAO), and large-scale structures have provided independent evidence for today's cosmic acceleration. In the

past there was a period called the matter-dominated epoch in which large-scale structures were formed due to the gravitational attraction of non-relativistic matter. After this epoch, the Universe entered the accelerating stage in which the energy density of dark energy dominates over that of non-relativistic matter. This paradigm has been consistent not only with SN Ia observations but also with other independent observations mentioned above. Riess, Schmidt, and Perlmutter won the Nobel Prize for Physics in 2011 for their first direct discoveries of the late-time cosmic acceleration.

While the notion of the accelerating Universe is now widely accepted, we did not yet identify the origin of dark energy. The vacuum energy appearing in particle physics behaves as the cosmological constant, but its energy scale is vastly larger than the observed dark energy scale. Instead, there have been other attempts to address the problem of dark energy. Broadly speaking, we can classify models of the late-time cosmic acceleration into two classes. One of them constitutes modified matter models in which specific sources of matter with negative pressure are introduced. Another constitutes modified gravity models in which the gravity sector is modified from general relativity. Different dark energy models leave different observational signatures, so it is possible to distinguish between them from observation.

In this book, I give a detailed account for both theoretical and observational aspects of dark energy for readers who are interested in joining this exciting research field. Since general relativity is a benchmark for studying physics of the expanding Universe, I provide basic tools of general relativity directly related to the study of dark energy. Next, I review the background cosmological dynamics by paying particular attention to the dynamics of inflation, reheating, radiation/matter eras. After reviewing the cosmic expansion history, I discuss the physics of late-time cosmic acceleration and explain how the property of dark energy is constrained from the distance measurements of SN Ia.

In modern cosmology, it is unarguably important to understand the evolution of cosmological perturbations to confront theoretical models with observations. For this purpose, I provide the basic framework of gauge-invariant cosmological perturbation theory in the presence of a fluid and a scalar field. My main prospect is to apply this general framework to dark energy, but I also compute the primordial power spectra of scalar and tensor perturbations generated during the stage of primordial inflation. Hence, this book can be useful for readers who are interested in observational predictions of the inflationary paradigm.

After the precise measurements of CMB temperature anisotropies by WMAP in 2003, the cosmology entered the golden age in which cosmological parameters are tightly constrained from the CMB data. Due to its importance, I provide detailed accounts for the theoretical calculation of the CMB angular power spectrum of temperature anisotropies. In particular, I study the evolution of linear perturbations from inflation to today and address how the existence of dark energy modifies the shape of the CMB power spectrum. Then, I show how the equation of state of dark

energy can be constrained from CMB observations. I also review the physics of BAO and discuss how the distance measurements of BAO place bounds on the property of dark energy.

The theory of cosmological perturbations is also applied to the growth of large-scale structures. I derive the matter power spectrum associated with galaxy clusterings and show the consistency of the dark energy paradigm with the observed galaxy power spectrum. I also provide basic frameworks to understand the physics of redshift-space distortions and weak lensing. This will be useful for placing tight constraints on the property of dark energy from future high-precision observations.

There are dark energy models already excluded from the joint data analysis of SN Ia, CMB, and BAO. In this book, I discuss theoretical aspects of models which are still consistent with current observations. The cosmological constant remains to be compatible with the data. From the theoretical side, there have been attempts to explain why the cosmological constant is so small or to sequester vacuum energy from the gravity sector. I review several approaches to address the cosmological constant problem.

Besides the cosmological constant, I study the cosmological dynamics for several representative dark energy scenarios including modified matter models (such as quintessence, k-essence) and modified gravity models (such as $f(R)$ gravity, Brans-Dicke theories, Galileons). Then I show that these models belong to a sub-class of most general scalar-tensor theories with second-order equations of motion — known as Horndeski theories. I derive the background and linear perturbation equations of motion in Horndeski theories and apply them to constrain each dark energy model from observations. I also discuss the construction of theories of a massive vector field coupled to gravity (called generalized Proca theories) and study their cosmological consequences.

In modified gravity theories, there are in general scalar or vector degrees of freedom that can propagate to mediate fifth forces with non-relativistic matter in regions of high density. I review two representative screening mechanisms of fifth forces — dubbed chameleon and Vainshtein mechanisms. I apply such screening mechanisms to concrete modified gravity theories like $f(R)$ gravity, Brans-Dicke theory, and Galileons. I also discuss how the parameter spaces in modified gravity theories are constrained from solar-system tests of gravity.

Finally, I review the approach of effective field theory (EFT) of dark energy based on the perturbative expansion of the Lagrangian expressed in terms of scalar quantities arising in the 3+1 decomposition of spacetime. This approach can accommodate not only Horndeski theories but also more general theories with equations of motion higher than second order. Since an efficient numerical code called the EFTCAMB has been developed to test for dark energy models with observational data, the EFT approach will be very helpful to constrain a vast class of dark energy models. The goal is to identify a theoretically consistent dark energy model best fitted to upcoming high-precision observational data.

This book is complementary in that both theoretical and observational aspects of dark energy are explained in detail. I made efforts such that the reader can follow physical logics and calculations step by step. After going through the book, I believe that the reader will already have sufficient expertise for working on concrete research topics relevant to dark energy. I hope that many people will join this exciting research field and help to reveal the origin of dark energy.

While I tried to eliminate typos and errors as much as possible, there may be some inappropriate parts I was not aware of. If readers find them, please feel free to write to shinji@rs.kagu.tus.ac.jp. I will try to reflect them in the next edition of the book.

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Frequently used notations

Symbol	Definition
t	Cosmic time
η	Conformal time: $\eta = \int a^{-1} dt$
a	Scale factor of the Universe (with the present value $a_0 = 1$)
$\mathcal{N}$	Number of e-foldings: $\mathcal{N} = \ln a$
N, N^i	lapse function, shift vector
$\dot{}$	Derivative with respect to t
$\prime$	Derivative with respect to η (unless otherwise stated)
z	Redshift ($z = a_0/a - 1$)
$g_{\mu\nu}$	Four-dimensional metric tensor
$q_{\mu\nu}$	Three-dimensional (3D) spatial metric tensor in the ADM formalism
$h_{\mu\nu}$	Tensor perturbations
$R_{\mu\nu}, G_{\mu\nu}$	Ricci tensor, Einstein tensor
R	Ricci scalar
$T_{\mu\nu}$	Energy-momentum tensor
$K_{ij}, \mathcal{R}_{ij}$	Extrinsic curvature, intrinsic curvature
d_A, d_L	Angular diameter distance, Luminosity distance
$H, \mathcal{H}$	Hubble parameter: $H = \dot{a}/a$, Conformal Hubble parameter $\mathcal{H} = aH$
H_0, h	Present Hubble parameter: $H_0 = 100 h \text{ km sec}^{-1} \text{ Mpc}^{-1}$
$E(z)$	Hubble parameter normalized by H_0 : $E(z) = H(z)/H_0$
Λ	Cosmological constant
ρ	(Energy) Density
P	Pressure
w_{DE}	Dark energy equation of state: $w = P_{\text{DE}}/\rho_{\text{DE}}$
w_{eff}	Effective or total equation of state: $w_{\text{eff}} = -1 - 2\dot{H}/(3H^2)$
$\mathcal{K}$	Spatial curvature
$\Omega^{(0)}$	Density parameter at the present epoch ($z = 0$)
c_s, c_t, c_v	Propagation speeds of scalar, tensor, vector perturbations
Ψ, Φ	Gravitational potentials
$\mathcal{V}, v$	Velocity potentials with the relation $\mathcal{V} = -a(v + B)$
T	Temperature
Θ	Temperature perturbations: $\Theta = \delta T/T$
k	Comoving wavenumber
$\mathcal{P}(k), P(k)$	Power spectra of perturbations with $\mathcal{P}(k) = k^3 P(k)/(2\pi^2)$
l	Spherical harmonic multipoles
C_ℓ	Multipole power spectrum
$\mathcal{R}$	Curvature perturbation in Chap. 6 and 3D Ricci scalar in Chap. 15
$\mathcal{R}_{\text{CMB}}$	CMB shift parameter
δ	Density contrast
ψ_{eff}	Weak lensing potential $\Phi - \Psi$
ϕ, χ	Scalar fields
X	Field kinetic energy: $X = -(1/2)g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi$
$\mathcal{L}$	Lagrangian density
Q	Coupling between a scalar field ϕ and non-relativistic matter
ω_{BD}	Brans–Dicke parameter

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Chapter 1

Introduction

The cosmology has made enormous progress after the construction of General Relativity (GR) in 1915. The theoretical predictions of GR — such as the existence of black holes and gravitational waves — have been directly/indirectly confirmed by observations. Now, we know that GR is sufficiently dependable to describe the gravitational law in the solar system.

In GR, the geometry of spacetime is directly related to a matter source through the Einstein equation. If we apply the Einstein equation to the cosmology in the presence of matter, the solutions with an expanding Universe naturally arise. At first Einstein did not support the idea of the cosmic expansion, so he added a term dubbed the cosmological constant Λ to realize a static Universe [1]. However, such a static configuration is unstable in that the existence of a small perturbation easily leads to either the expanding or the contracting Universe. In 1929, Hubble discovered that the Universe is expanding from the observations of distant galaxies [2], after which Einstein abandoned the idea of the static Universe.

In 1946, Gamov [3] proposed the notion of the Big Bang cosmology where the expanding Universe has cooled down from the initial hot and high-density state. According to the Big Bang cosmology, the creation of elements occurred as the temperature of photons decreased. In fact, the light nuclei like deuterium and helium were formed in the early cosmological epoch with the temperature around $T = 10^9$ K. This process is called the Big Bang Nucleosynthesis (BBN). The amount of light nuclei predicted by BBN exhibited good agreement with their observed primordial abundance.

If the Big Bang cosmology were correct, the early Universe was dominated by the black body radiation in a state of thermal equilibrium. In 1965, Penzias and Wilson [4] coincidentally discovered the cosmic microwave background radiation by observing microwaves from the sky with a Horn Antenna. The microwaves arrived from all parts of the sky with nearly same temperature ($T \approx 3$ K). This was a remnant of the black body radiation in the early Universe, which was dubbed the

Cosmic Microwave Background (CMB). The CMB photons began to stream freely after free electrons were captured by light atomic nuclei like hydrogen and helium. This decoupling occurred around the temperature $T \approx 3000$ K. Penzias and Wilson observed the CMB photons emitted from the decoupling epoch. Since the scale factor of the Universe increased about 10^3 times from the decoupling era to today, the black body radiation observed by us has the temperature $T \approx 3$ K (i.e., inversely proportional to the scale factor). The discovery of CMB provided the strong evidence for the Big Bang cosmology.

In 1989, the COBE satellite was launched for the purpose of measuring the energy distribution of CMB photons precisely. In fact, the energy distribution measured by COBE in 1992 showed excellent agreement with the black body radiation with the average temperature $T = 2.7$ K [5]. Moreover, the COBE measured the existence of small temperature fluctuations δT at large scales. The CMB temperature anisotropies, which are of the order of $\delta T/T \approx 10^{-5}$, are responsible for the origin of large-scale structures in the Universe. The galaxies were formed due to the gravitational clustering of primordial density perturbations.

Independent of the discovery of CMB temperature anisotropies, the inflationary paradigm was proposed in the early 1980s to address several problems of the Big Bang cosmology [6–9]. The Big Bang cosmology is based upon the decelerated expansion from the Big Bang to today. In this case, the causal region in which the information is transmitted by light (called the particle horizon) at the decoupling epoch is much smaller than today’s particle horizon. However, the CMB photons reached us from all parts of the sky with almost the same temperature. This problem, which is dubbed the horizon problem, is difficult to be addressed in the Big Bang cosmology. Observationally, it is also known that spatial geometry of today’s Universe is nearly flat [10]. Since the contribution of spatial curvature to the Einstein equation increases with the decelerated cosmic expansion, it is also difficult to explain why the present Universe is almost flat in the context of the Big Bang cosmology. This is known as the flatness problem.

If the accelerated expansion (inflation) occurred in the very early Universe, it is possible to resolve both horizon and flatness problems. In fact, the vacuum energy arising in quantum field theory can drive a rapid cosmic acceleration. Moreover, the tiny vacuum fluctuations are stretched over super Hubble scales during inflation. This can be responsible for the origin of CMB temperature anisotropies. Theoretical calculations showed that the primordial power spectrum generated during inflation is nearly scale-invariant, i.e., the amplitude of perturbations hardly depends on scales [11–14]. Although the COBE satellite measured the CMB temperature anisotropies only on large scales, the observed power spectrum was consistent with the theoretical prediction.

In 1998, the first evidence for today’s cosmic acceleration was reported independently by Riess *et al.* [15] and Perlmutter *et al.* [16] from the measurements of Supernovae type Ia (SN Ia). This surprising discovery showed that the Universe

entered a stage of the accelerated expansion after the matter-dominated epoch. The standard matter like baryons, leptons, and photons only gives rise to the decelerated cosmic expansion, so we need an additional energy source for explaining the SN Ia data. This unknown energy source, which is dubbed dark energy [17], constitutes about 70% of the total energy budget of today's Universe.

After 1998, the existence of dark energy has also been confirmed by other independent observational data such as CMB [18] and Baryon Acoustic Oscillations (BAO) [19]. In particular, the WAMP satellite was launched in 2001 for the precise measurement of CMB temperature anisotropies including small-scale regions uncovered by the COBE measurement. The WMAP observations showed that today's Universe is composed of dark energy (about 70%), dark matter (about 25%), atoms (about 5%), and radiation (about 0.01%) [18]. Dark matter is another unknown component responsible for structure formation. Dark matter clusters are due to gravitational instability, while dark energy has an effective negative pressure responsible for cosmic acceleration.

The simplest candidate for dark energy is the so-called cosmological constant Λ . The property of the cosmological constant is similar to the vacuum energy, whose energy density is constant in time. If the cosmological constant is related to the vacuum energy appearing in particle physics, its energy scale is enormously larger than the observed dark energy scale ($\rho_{\text{DE}}^{(0)} \simeq 10^{-47} \text{ GeV}^4$) [20]. Hence one needs to find a mechanism to obtain a tiny value of Λ consistent with observations. Much effort has been made in this direction, but we are still on the way of resolving the cosmological constant problem.

The first step toward understanding the property of dark energy is to clarify whether it is a simple cosmological constant or whether it originates from other sources dynamically changing in time [21–29]. The dynamical dark energy models can be distinguished from the cosmological constant by the evolution of $w_{\text{DE}} = P_{\text{DE}}/\rho_{\text{DE}}$, where ρ_{DE} is the energy density and P_{DE} is the pressure of dark energy. The scalar field models of dark energy such as quintessence [30–36] and k-essence [37–39] predict a wide variety of variations of w_{DE} , but there have been no strong observational evidence that such models are favored over the cosmological constant. Moreover, the scalar-field potentials need to be sufficiently flat such that the field evolves slowly to drive today's cosmic acceleration. This demands that the field mass is extremely small ($m_\phi \simeq 10^{-33} \text{ eV}$) relative to typical mass scales appearing in particle physics. However, as we will discuss in this book, it is not entirely hopeless to construct viable scalar-field dark energy models in the framework of particle physics.

There are other classes of dark energy models based on the modification of GR. If we modify the gravitational law from GR, the breaking of gauge symmetries present in GR generally gives rise to additional propagating degrees of freedom. In $f(R)$ gravity, where the Lagrangian f is a function of the Ricci scalar R , for example, there exists a scalar degree of freedom with the gravitational origin [6].

This gravitational scalar, which is called the scalaron, can drive today’s cosmic acceleration, depending on the functional forms of $f(R)$ [40–43].

It is known that $f(R)$ gravity belongs to a class of scalar–tensor theories called Brans–Dicke theories [44]. In Brans–Dicke theories, there is a coupling between a scalar field ϕ and gravity in the form ϕR . One can also consider more general derivative couplings where the field kinetic energy X is coupled to the Ricci scalar R and the Einstein tensor $G_{\mu\nu}$. One such derivative coupling model is Galileons [45–48], whose equations of motion respect the galilean symmetry $\partial_\mu\phi \rightarrow \partial_\mu\phi + b_\mu$ in the limit of Minkowski spacetime. The Lagrangian of Galileons is constructed to keep the equations of motion up to second order to avoid a ghost-like Ostrogradski instability associated with a Hamiltonian unbounded from below. The most general scalar–tensor theories with second-order equations of motion, which are the extension of Galileons, are known as Horndeski theories [49]. Horndeski theories cover a wide variety of modified gravity theories proposed in the literature. It is also possible to construct theories with a vector field coupled to gravity [50–52] or theories with a massive graviton [53].

In addition to the said models, there are also attempts to explain the cosmic acceleration without resorting to an unknown dark component. The Lemaître–Tolman–Bondi (LTB) void scenario is a representative model in which an apparent accelerated expansion is induced by large spatial inhomogeneities [54–56]. However, the LTB model was ruled out from the joint data analysis of the BAO and SN Ia data at high confidence [57]. In this book, we will mainly focus on theoretically consistent models of dark energy which have not yet been excluded in current observations.

To distinguish between a host of dark energy models proposed in the literature, it is important to study their observational signatures. In particular, the equation of state w_{DE} is a key quantity for describing the property of dark energy at the background level. The cosmological constant corresponds to the value $w_{\text{DE}} = -1$, whereas other dynamical dark energy models generally predict the time-varying equation of state. Modified matter models like quintessence and k-essence usually lead to w_{DE} larger than -1 , while modified gravity models can give rise to w_{DE} smaller than -1 . If the evolution of w_{DE} is very tightly constrained from future high-precision observations, it should be possible to approach the best model of dark energy. The cosmological constant has been overall consistent with numerous observational data, but the deviation of w_{DE} from -1 can also be allowed. We will study the evolution of w_{DE} for theoretically consistent dark energy models and discuss how the models can be observationally distinguished from each other by the background cosmic expansion history.

For constraining dark energy models from the measurements of large-scale structures, weak lensing, and CMB etc., it is important to study the development of spatial inhomogeneities on the isotropic and homogenous Friedmann–Lemaître–Robertson–Walker (FLRW) background. In doing so, we need to understand the

evolution of cosmological perturbations in GR and also in modified gravity theories. Since the theory of cosmological perturbations is exploited to confront any dark energy models with observations, we will give a detailed account for its basis. The book also covers topics like primordial perturbations generated during inflation, CMB temperature anisotropies, BAO, matter power spectra, red-shift space distortions, and weak lensing.

We will also discuss observational signatures of theories beyond GR and provide prescriptions to distinguish numerous dark energy models from observations associated with the growth of spatial inhomogeneities. Especially, the effective field theory (EFT) of dark energy [58–65] is a powerful tool to deal with a wide range of modified gravitational theories including Horndeski theories and its extensions. We will provide a basic theoretical framework of the EFT of dark energy, paying particular attention to the connection with each modified gravity theory. This approach is useful for constraining a host of dark energy models from observations.

If there exist additional scalar or vector degrees of freedom to those appearing in Standard Model (SM) of particle physics, they can interact with SM particles. This is particularly the case for modified gravity theories, in which additional degrees of freedom have direct couplings to gravity. Such couplings can mediate fifth forces, which were not yet observed in local gravity experiments. In other words, the gravitational law in the solar system is close to the prediction of GR. Even if some degrees of freedom in modified gravitational theories can explain the cosmic acceleration at large distances, the same theories need to recover the gravitational law close to that of GR at small distances. There are several mechanisms for screening the propagation of fifth forces in local regions of the Universe [66–68]. We will review how screening mechanisms are at work in concrete models of the late-time cosmic acceleration.

This book is organized as follows.

- In Chap. 2, we review historical findings of the expanding Universe: the Hubble’s discovery and the CMB black body radiation.
- In Chap. 3, we provide basic tools of GR required for studying physics of dark energy.
- In Chap. 4, we review the cosmic expansion history from the inflationary epoch to today.
- In Chap. 5, we explain observational evidence for the late-time cosmic acceleration at the background level including SN Ia measurements.
- In Chap. 6, we provide basics of cosmological perturbation theory and apply them to the derivation of primordial power spectra generated during inflation.
- In Chap. 7, we study the evolution of cosmological perturbations from the primordial era to today and analytically estimate the angular power spectrum of CMB temperature anisotropies.

- In Chap. 8, we discuss how the property of dark energy can be constrained from measurements associated with the development of inhomogeneities such as CMB, galaxy clusterings, BAO, and weak lensing.
- In Chap. 9, we highlight several approaches to trying to solve the cosmological constant problem.
- In Chap. 10, we give a detailed account for modified matter models of dark energy, including quintessence, k-essence, and coupled dark energy.
- In Chap. 11, we review the background cosmology in several representative modified gravity theories, including $f(R)$ gravity, Brans–Dicke theories, and Galileons.
- In Chap. 12, we derive linear perturbation equations of motion in Horndeski theories and apply them to concrete modified gravity theories.
- In Chap. 13, we review dark energy models based on massive vector fields with derivative interactions — dubbed generalized Proca theories.
- In Chap. 14, we discuss two screening mechanisms of fifth forces (chameleon and Vainshtein mechanisms) in Horndeski and generalized Proca theories.
- In Chap. 15, we provide a basic framework for the EFT of dark energy. We pay particular attention to relations with concrete theories (including Horndeski theories, its extensions, Hořava–Lifshitz gravity) to confront them with observations.
- Chap. 16 is devoted to the conclusion.

Throughout the book, we adopt the metric signature $(-, +, +, +)$. For fundamental physical constants, we use c for the speed of light, h for the Planck constant, k_B for the Boltzmann constant, and G for the gravitational constant. Their numerical values are

$$c = 2.9979 \times 10^8 \text{ m s}^{-1}, \quad (1.1)$$

$$h = 6.6261 \times 10^{-34} \text{ J s} = 4.1357 \times 10^{-15} \text{ eV s}, \quad (1.2)$$

$$k_B = 1.3806 \times 10^{-23} \text{ J K}^{-1} = 8.6173 \times 10^{-5} \text{ eV K}^{-1}, \quad (1.3)$$

$$G = 6.6738 \times 10^{-11} \text{ kg}^{-1} \text{ m}^3 \text{ s}^{-2}. \quad (1.4)$$

The reduced Planck constant is defined by

$$\hbar \equiv \frac{h}{2\pi} = 1.0546 \times 10^{-34} \text{ J s} = 6.5821 \times 10^{-16} \text{ eV s}. \quad (1.5)$$

The Planck mass m_{pl} , the Planck time t_{pl} , and the Planck length ℓ_{pl} are given, respectively, by

$$\ell_{\text{pl}} = \sqrt{\frac{\hbar G}{c^3}} = 1.6162 \times 10^{-35} \text{ m}, \quad (1.6)$$

$$t_{\text{pl}} = \sqrt{\frac{\hbar G}{c^5}} = 5.3911 \times 10^{-44} \text{ s}, \quad (1.7)$$

$$m_{\text{pl}} = \sqrt{\frac{\hbar c}{G}} = 2.1765 \times 10^{-8} \text{ kg} = 1.2209 \times 10^{19} \text{ GeV}/c^2. \quad (1.8)$$

We also introduce the reduced Planck mass, as

$$M_{\text{pl}} = \frac{m_{\text{pl}}}{\sqrt{8\pi}} = 2.4353 \times 10^{18} \text{ GeV}/c^2. \quad (1.9)$$

The natural unit corresponds to $c = \hbar = k_B = 1$, in which case we have

$$\ell_{\text{pl}} = t_{\text{pl}} = \frac{1}{m_{\text{pl}}} = \frac{1}{\sqrt{8\pi}M_{\text{pl}}} = \sqrt{G}. \quad (1.10)$$

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Chapter 2

Expanding Universe

2.1. Hubble–Lemaître’s law

A light emitted from a source travels to us with the finite speed $c = 2.9979 \times 10^8 \text{ m s}^{-1}$. Hence there is a time delay between the moment at which the light is emitted and the moment at which it is detected by an observer. Then we can observe objects as they were when the Universe was much younger than it is now. The construction of a telescope at the Mount Wilson observatory in the early 1900s opened up a possibility for observing stars outside our galaxies (which are more than 10^5 light years away from us).

In 1929, Hubble discovered from the observations of distant galaxies (including the Andromeda galaxy) that the Universe is expanding [1]. This is based on the fact that the wavelength of light is stretched by the expansion of the Universe through the Doppler effect. Suppose that the light emitted from a source has the wavelength λ at cosmic time t and that the same light is observed with the wavelength λ_0 today (at time t_0). The physical wavelength is stretched in proportion to a scale factor of the Universe (which depends on the cosmic time t). Provided that the expansion of the Universe is isotropic, the scale factor $a(t)$ evolves in the same way along three spatial dimensions.

We define the redshift z of an object, as

$$z \equiv \frac{\lambda_0}{\lambda} - 1 = \frac{a_0}{a(t)} - 1, \quad (2.1)$$

where a_0 is the value of a today. The present epoch corresponds to $z = 0$. As we go back to the past, z gets larger with the decrease of $a(t)$. The redshift is related to the recession velocity v of the source. From the Doppler effect of special relativity [2], the ratio λ_0/λ reads

$$\frac{\lambda_0}{\lambda} = \sqrt{\frac{c+v}{c-v}}, \quad (2.2)$$

which is larger than 1. If $v \ll c$, then the approximate relation $z \simeq v/c$ holds from Eqs. (2.1) and (2.2). By measuring λ_0 and λ observationally, the redshift z and the recession velocity v are known accordingly.

On the isotropic expanding cosmological background, a physical distance $\mathbf{r}$ between source and observer is related to a comoving distance $\mathbf{x}$, as

$$\mathbf{r} = a(t)\mathbf{x}. \quad (2.3)$$

The coming distance $\mathbf{x}$ corresponds to the distance whose coordinate value does not change along the cosmic expansion. If the source has a peculiar velocity of its own, $\mathbf{x}$ is subject to change.

Taking the time derivative of Eq. (2.3), we obtain the relation

$$\dot{\mathbf{r}} = H\mathbf{r} + a\dot{\mathbf{x}}, \quad (2.4)$$

where a dot represents a derivative with respect to t , and

$$H \equiv \frac{\dot{a}(t)}{a(t)}. \quad (2.5)$$

The quantity (2.5) is called the Hubble parameter, which characterizes the expansion rate of the Universe. The velocity component along the line-of-sight direction from the observer to the source is given by $v = \dot{\mathbf{r}} \cdot \mathbf{r}/r$, where $r = |\mathbf{r}|$. On using Eq. (2.4), it follows that

$$v = Hr + a\dot{\mathbf{x}} \cdot \frac{\mathbf{r}}{r}. \quad (2.6)$$

The contribution $v_H \equiv Hr$ arises due to the cosmic expansion, which is positive on the expanding background ($H > 0$). Meanwhile, the contribution $v_p \equiv a\dot{\mathbf{x}} \cdot \mathbf{r}/r$ corresponds to the line-of-sight component of the peculiar velocity of the object. Depending on the direction of the velocity $\dot{\mathbf{x}}$, the value v_p can be either positive or negative.

For nearby sources from the Earth the distance r is small, so the condition $v_H \ll |v_p|$ is satisfied. In this case, v can be either positive or negative depending on the direction of peculiar velocities. For far distant sources, v_H overwhelms $|v_p|$, so that the objects recede away from us. From the observations of Cepheid variable stars in the Andromeda galaxy, Hubble found that the galaxy is moving away from us. The Cepheid variable star is an object whose luminosity periodically changes in time. Since there is a specific relation between its period T and the maximum luminosity M [3], it is possible to estimate M by observing T . Comparing M with the observed luminosity m , Hubble measured the distance to distant galaxies [1].

The recession velocity v of the galaxy measured by Hubble is at most 10^6 m s^{-1} , i.e., $v \lesssim 10^{-2}c$. In this case, the velocity is known as $v \simeq cz = c(\lambda_0/\lambda - 1)$ from the redshift measurements. Ignoring the contribution of the peculiar velocity in Eq. (2.6) relative to Hr and using the approximation that H is approximately equivalent to today's expansion rate H_0 (called the Hubble constant) for $z \ll 1$, we obtain

$$v \simeq H_0 r. \quad (2.7)$$

In 1929, Hubble plotted the observational data of v and r for Cepheids and showed that they can be fitted by the linear relation (2.7). In 1927, Lemaître already derived the same relation as Eq. (2.7) in a paper written in French [5]. Reflecting this fact, we call the relation (2.7) the Hubble–Lemaître’s law.

In his first analysis, Hubble underestimated the distance to Cepheids by one order of magnitude smaller than its correct value and obtained $H_0 \approx 500 \text{ km s}^{-1} \text{ Mpc}^{-1}$ from a tangent of the line in the v – r plane (called the Hubble diagram). Here, 1 Mpc corresponds to the distance

$$1 \text{ Mpc} = 10^6 \text{ pc} = 3.0857 \times 10^{24} \text{ cm}. \quad (2.8)$$

According to today’s more precise measurements, the Hubble constant H_0 is about $70 \text{ km s}^{-1} \text{ Mpc}^{-1}$. Usually, this is expressed in the form

$$H_0 = 100 h \text{ km s}^{-1} \text{ Mpc}^{-1} = (3.0857 \times 10^{17} \text{ s})^{-1} h, \quad (2.9)$$

where h is a dimensionless constant. In Fig. 2.1, we plot the observational data of v and r for Cepheids observed by the Hubble Key project [6]. The dimensionless constant h is constrained to be $h = 0.72 \pm 0.08$, where ± 0.08 is the error. The analyses of WMAP [7] and Planck [8] based on the observational data of CMB temperature anisotropies showed that h is constrained to be $h = 0.700 \pm 0.022$ and $h = 0.673 \pm 0.012$, respectively.

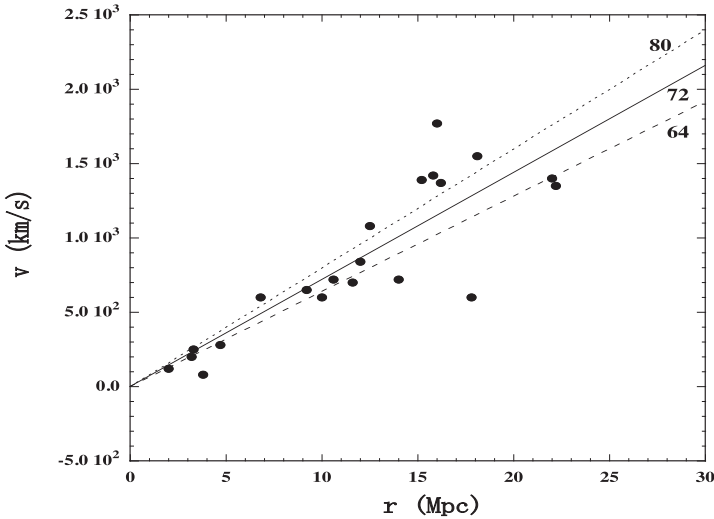


Fig. 2.1. Hubble diagram derived from the data of Ref. [4]. The horizontal and vertical axes correspond to the distance r and the velocity v of observed galaxies. Several numbers in the figure represent tangents of three lines with the unit $\text{km s}^{-1} \text{ Mpc}^{-1}$. We do not plot error bars of the data.

We note that H_0^{-1} has the unit of time. As we will see in Sec. 5.1, H_0^{-1} is of the same order as the age of our Universe. Then, the distance

$$cH_0^{-1} = 2998 h^{-1} \text{ Mpc} \approx 10^{28} \text{ cm} \quad (2.10)$$

can be regarded as an observable size of the today's Universe. In the Hubble's observations, the redshift was in the range $z \ll 1$, but in current observations we can measure objects (like SN Ia) with the redshift larger than 0.5. In such cases, the approximation that $H(z)$ is equivalent to H_0 is no longer dependable. The late-time cosmic acceleration was discovered by measuring the high-redshift SN Ia in the range $z \gtrsim 0.5$ [9, 10]. In Sec. 5.3, we will see how the Hubble diagram is modified for objects with high redshifts.

2.2. Cosmic microwave background (CMB)

In 1964, Penzias and Wilson were mapping signals from the Milky Way by using a large horn antenna. They found a low and steady signal that persisted even after eliminating all possible sources of interference. This signal, which came from all parts of the sky at all times, was the first discovery of CMB [11]. The discovery of CMB provided us with independent observational evidence for the Big Bang cosmology. According to the Big Bang paradigm the Universe was initially in a hot and dense state, but the temperature decreased along with the expansion of the Universe. The CMB corresponds to ancient lights emitted about 380,000 years after the Big Bang in a state of thermal equilibrium (called the black body radiation) with the temperature about 3000 K. In the present Universe, the temperature of the CMB photon is about 3 K.

The most ancient Universe observed by light is the so-called decoupling epoch at which the photon could start to move freely. Before the decoupling, photons were frequently scattered by the electron, so the light did not reach us. After the temperature of the Universe decreased below 3000 K, electrons started to be captured by protons and other nuclei to form atoms. Then, after the decoupling epoch, photons freely streamed without being scattered by free electrons. The CMB is the black body radiation emitted at the decoupling time with the redshift $z \simeq 1090$.

In 1989, the COBE satellite was launched for the purpose of measuring precisely the energy distribution of CMB photons. In a state of thermal equilibrium with the black-body temperature T , the number density of photons with the frequency between ν and $\nu + d\nu$ is given by the distribution function

$$n(\nu, T) d\nu = \frac{8\pi}{c^3} \frac{\nu^2}{\exp[h\nu/(k_B T)] - 1} d\nu, \quad (2.11)$$

where k_B is Boltzmann constant and h is the Planck constant.

Let us consider a CMB photon with the frequency ν_* and the wavelength λ_* at the decoupling epoch (with the scale factor a_*). At the time when the scale

factor grows to a , the frequency ν and the wavelength λ of the photon obey $\nu_*/\nu = \lambda/\lambda_* = a/a_*$. After the decoupling epoch with temperature T , we write the photon's number density as $\tilde{n}(\nu, T)$. Then, the conservation of photon numbers leads to

$$a_*^3 n(\nu_*, T_*) d\nu_* = a^3 \tilde{n}(\nu, T) d\nu. \quad (2.12)$$

Applying Eq. (2.11) to the left hand side of Eq. (2.12) and using the relation $\nu_* = (a/a_*)\nu$, we can derive $\tilde{n}(\nu, T)$. In doing so, we define the temperature after the decoupling epoch, as

$$T = T_* \frac{a_*}{a}. \quad (2.13)$$

Then, the resulting number density is given by

$$\tilde{n}(\nu, T) d\nu = \frac{8\pi}{c^3} \frac{\nu^2}{\exp[h\nu/(k_B T)] - 1} d\nu. \quad (2.14)$$

This shows that, as long as one defines the temperature as Eq. (2.13) after the decoupling, the number density of CMB photons preserves the structure of black body radiation. As we will see later in Sec. 4.4, the temperature of radiation in a state of thermal equilibrium also decreases as $T \propto a^{-1}$.

The energy density ε of a black body with the temperature T and the frequency between ν and $\nu + d\nu$ obeys the Planck distribution

$$\varepsilon(\nu, T) d\nu = h\nu n(\nu, T) d\nu = \frac{8\pi h}{c^3} \frac{\nu^3}{\exp[h\nu/(k_B T)] - 1} d\nu. \quad (2.15)$$

For a given temperature T , we have that $\varepsilon(\nu \rightarrow 0) = 0$ and $\varepsilon(\nu \rightarrow \infty) = 0$. The energy density has a maximum value at $\nu \simeq 2.82 k_B T/h$. After the decoupling epoch, we define the energy density as $\tilde{\varepsilon}(\nu, T) = h\nu \tilde{n}(\nu, T)$, where T and $\tilde{n}(\nu, T)$ are given, respectively, by Eqs. (2.13) and (2.14). Then, the energy distribution $\tilde{\varepsilon}(\nu, T) d\nu$ is of the same form as Eq. (2.15) in the thermal equilibrium. The CMB photons should be observed with the energy density $\varepsilon(\nu_0, T_0)$, where ν_0 and T_0 are today's values of ν and T respectively. In fact, the theoretical prediction of black body radiation showed excellent agreement with the CMB data observed by COBE (see Fig. 2.2). The COBE data constrained the temperature of the present Universe to be

$$T_0 = 2.725 \pm 0.002 \text{ K}. \quad (2.16)$$

Introducing the dimensionless variable $x = h\nu/(k_B T)$ and integrating the Planck distribution (2.15) over all frequencies, the total energy density reads

$$\varepsilon_\gamma(T) = \int_0^\infty \varepsilon(\nu, T) d\nu = \frac{(k_B T)^4}{\pi^2 (\hbar c)^3} \int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^2}{15} \frac{k_B^4}{(\hbar c)^3} T^4, \quad (2.17)$$

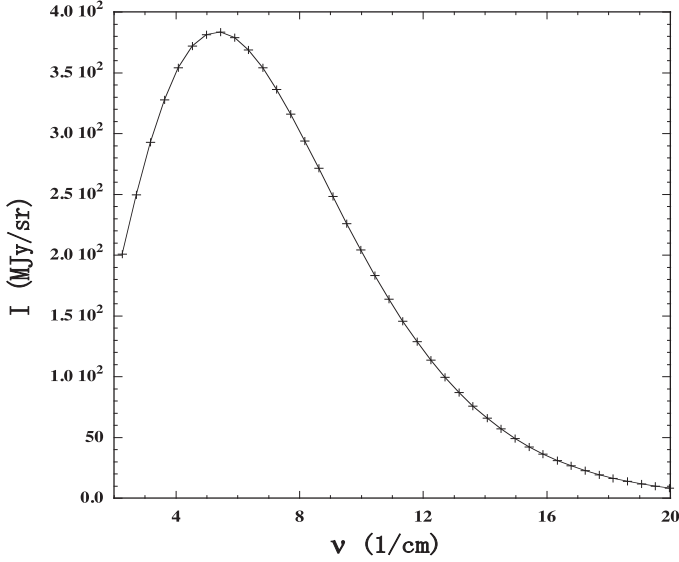


Fig. 2.2. Theoretical prediction of the black-body radiation spectrum with today's temperature $T_0 = 2.725$ K (solid curve). The horizontal and vertical axes show the frequency ν and the intensity I of photons, respectively. The COBE data [12] are shown as the “+” symbol.

where $\hbar = h/(2\pi)$ is the reduced Planck mass. Today's value of ε_γ corresponding to the temperature $T_0 = 2.725$ K is given by

$$\varepsilon_\gamma^{(0)}(T_0) = 4.17 \times 10^{-20} \text{ J cm}^{-3}. \quad (2.18)$$

As we will see in Sec. 4.3, this energy density is less than 0.01 % of the total energy density of the present Universe.

The COBE satellite not only confirmed the Big Bang cosmology, but also it measured CMB temperature anisotropies of the order of $\delta T/T \sim 10^{-5}$ [12]. By measuring CMB temperature anisotropies precisely, it is possible to extract useful information for cosmological parameters. In 2001, the WMAP satellite was launched for this purpose, which opened up a new era of high-precision cosmology. We will discuss the physics of CMB temperature anisotropies in Chap. 7.

2.3. Newtonian picture of the expansion of the Universe

In the context of Newtonian gravity, it is possible to describe the cosmic expansion in the Universe dominated by a dust particle. Here, the dust particle means non-relativistic matter with a negligible pressure relative to its energy density. Considering a setup of homogenous and isotropic cosmological backgrounds, one can take a sphere (radius a) with its central point O. The mass of the sphere is given by $M = \rho V$, where ρ is the density of non-relativistic matter and $V = 4\pi a^3/3$ is the sphere volume. If one considers a point particle (mass m) moving along the radial

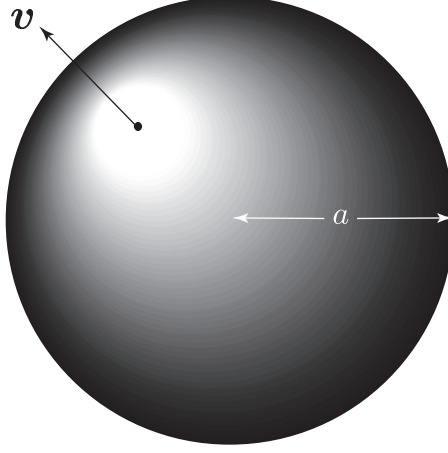


Fig. 2.3. A point particle of mass m moving along the radial direction (velocity v) on the surface of a sphere with mass M and radius a .

direction with the surface of sphere, the gravitational force exerted on this particle is given by GmM/a^2 (see Fig. 2.3 for the illustration). Then, Newton's equation of motion at time t is given by

$$m\ddot{a} = -G\frac{mM}{a^2}, \quad (2.19)$$

so that

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}\rho. \quad (2.20)$$

This shows that, for $\rho > 0$, the Universe exhibits the decelerated expansion ($\ddot{a} < 0$). Equation (2.20) is valid for non-relativistic matter, but for the matter with a non-negligible pressure, the right hand side of Eq. (2.20) is subject to change. As we will see in Chap. 3, the effect of pressure can be accommodated in the framework of GR. This is important for discussing the cosmological evolution in the radiation era or in the epoch dominated by dark energy. The effect of dark energy corresponds to a negative pressure against gravity, which gives rise to a positive term on the right hand side of Eq. (2.20). This leads to the accelerating Universe characterized by $\ddot{a} > 0$.

In the following, we will derive the evolution of the scale factor in the Universe dominated by non-relativistic matter. Multiplying Eq. (2.19) by the particle velocity v ($= \dot{a}$) and integrating it with respect to t , it follows that

$$\frac{1}{2}m\dot{a}^2 - G\frac{mM}{a} = E, \quad (2.21)$$

where E is an integration constant. Equation (2.21) shows that the sum of kinetic energy $m\dot{a}^2/2$ and potential energy $-GmM/a$ is conserved. For $E > 0$, the particle

goes to infinity ($a \rightarrow \infty$) with $\dot{a}^2 > 0$, whereas for $E < 0$, the velocity $\dot{a}$ reaches 0 at a point with the scale factor $a_* = -GmM/E$. If $E = 0$, then the particle marginally goes to infinity with the velocity $\dot{a} \rightarrow 0$ as $a \rightarrow \infty$.

Introducing a constant $\mathcal{K}$ related to the total energy E as $E = -\mathcal{K}mc^2/2$, Eq. (2.21) can be written in the form

$$H^2 - \frac{8\pi G}{3}\rho = -\frac{\mathcal{K}c^2}{a^2}, \quad (2.22)$$

where H is the Hubble expansion rate defined by Eq. (2.5). As we will see in Sec. 4.2, the constant $\mathcal{K}$ is related to the spatial curvature of the Universe. The case $\mathcal{K} < 0$ (i.e., $E > 0$) corresponds to the open Universe with an infinite volume, whereas the case $\mathcal{K} > 0$ to the closed Universe with a finite radius a_* . The case $\mathcal{K} = 0$ corresponds to the flat Universe with an infinite volume. From the CMB observations, it is known that the present Universe is close to the flat state [7, 8]. This is attributed to the fact that the accelerated expansion called inflation occurred in the very early Universe (which we will discuss in Sec. 4.6).

The mass $M = \rho V$ is conserved in the Universe dominated by non-relativistic matter, so the matter density decreases as

$$\rho = Ca^{-3}, \quad (2.23)$$

where C is a constant. Substituting Eq. (2.23) into Eq. (2.22) with $\mathcal{K} = 0$, it follows that

$$a^{1/2} \dot{a} = A, \quad (2.24)$$

where $A = \sqrt{8\pi GC/3}$ and the expanding branch ($H > 0$) is chosen here. Integrating Eq. (2.24) with respect to t , we obtain the solution

$$a = \left[\frac{3}{2}(At + B) \right]^{2/3}, \quad (2.25)$$

where B is an integration constant. After a sufficiently long period, the scale factor grows as

$$a \propto t^{2/3}, \quad (2.26)$$

which corresponds to the decelerated expansion.

In GR, the equation same as (2.22) follows from one of Einstein equations. As we will see in Sec. 4.2, Eq. (2.22) is also valid in the Universe dominated by a matter source with a non-negligible pressure (radiation or dark energy). However, the matter conservation equation (2.23) is subject to change in the presence of pressure. This leads to modifications to the evolution of ρ and a . To address the cosmological evolution in such cases, we will first review the basics of GR in Chap. 3 and then apply them to the background expansion history of the Universe in Chap. 4.

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Chapter 3

General Relativity

Einstein developed two theories of relativity in the early 20th century: special relativity and general relativity. Special relativity is a relativistic theory of spacetime between two inertial frames with non-accelerating observers. General Relativity (GR) is a geometric theory of gravitation constructed by extending special relativity to include acceleration in the theory [1]. Einstein developed the theory of GR by assuming an equivalence principle, under which a freely falling frame of reference is physically indistinguishable from an inertial frame. In other words, a freely falling observer in an elevator cannot distinguish whether he is accelerating under the influence of gravity or he is in a local inertial frame without gravity. If the equivalence principle holds, the inertial mass and the gravitational mass are equivalent to each other. According to local gravity experiments in the solar system, it is known that the equivalence principle between inertial and gravitational masses holds in high precision [2].

Unlike Newton's law of gravitation, GR can be applied to the physics of strong gravitational backgrounds, e.g., the early Universe, neutron stars, black holes, etc. In GR, the spacetime geometry is directly related to the matter sector through Einstein equations. For example, the cosmological evolution (geometry), which depends on matter species in the Universe, is known by solving Einstein equations on a time-dependent background. In this chapter, we will review the basics of GR for the purpose of applying them to the cosmological expansion history and the growth of inhomogeneities in later chapters.

3.1. Metric tensor

Let us consider the four-dimensional spacetime with the coordinate $x^\mu = (x^0, x^1, x^2, x^3)$ with $x^0 = ct$. The infinitesimal line element around each spacetime point x^μ is given by

$$ds^2 = g_{\mu\nu}(x)dx^\mu dx^\nu, \quad (3.1)$$

where $g_{\mu\nu}(x)$ is the metric tensor. Here and in the following, we use the notation that variables containing same lower and upper indices are summed over, e.g., $ds^2 = g_{00}dx^0dx^0 + g_{01}dx^0dx^1 + \cdots + g_{33}dx^3dx^3$. Since $g_{\mu\nu}(x)$ is defined as a symmetric tensor satisfying $g_{\mu\nu} = g_{\nu\mu}$, there are in general ten independent components. We use Greek indices to denote space and time components of a tensor, whereas Latin indices are used to denote spatial components.

Besides x^μ , let us take another coordinate $\tilde{x}^\mu$ with the metric tensor $\tilde{g}_{\mu\nu}(\tilde{x})$. The transformation between two coordinates is given by

$$d\tilde{x}^\alpha = \frac{\partial \tilde{x}^\alpha}{\partial x^\mu} dx^\mu. \quad (3.2)$$

Since the line element ds^2 does not depend on the choice of coordinates, it follows that $g_{\mu\nu}(x)dx^\mu dx^\nu = \tilde{g}_{\alpha\beta}(\tilde{x})d\tilde{x}^\alpha d\tilde{x}^\beta$. On using the relation (3.2), we obtain

$$g_{\mu\nu}(x) = \frac{\partial \tilde{x}^\alpha}{\partial x^\mu} \frac{\partial \tilde{x}^\beta}{\partial x^\nu} \tilde{g}_{\alpha\beta}(\tilde{x}). \quad (3.3)$$

According to the equivalence principle, it is possible to transform a frame on curved backgrounds with the coordinate x to a locally inertial frame described by the coordinate $\tilde{x}$. In this locally inertial frame, the metric tensor is equivalent to that in the flat (Minkowski) spacetime, i.e.,

$$\tilde{g}_{\alpha\beta}(\tilde{x}) = \eta_{\alpha\beta} = \text{diag}(-1, 1, 1, 1), \quad (3.4)$$

where “diag” represents diagonal components. Taking the determinant of Eq. (3.3), we find

$$\det(g_{\mu\nu}) = - \left| \frac{\partial \tilde{x}}{\partial x} \right|^2. \quad (3.5)$$

Since the quantity $J = |\partial \tilde{x} / \partial x|$ corresponds to a Jacobian, it follows that

$$J = \sqrt{-g}, \quad (3.6)$$

where $g = \det(g_{\mu\nu})$ is a determinant of the metric tensor. The volume element $d^4x = dx^0dx^1dx^2dx^3$ is transformed to the one in the locally inertial frame, as $d^4\tilde{x} = Jd^4x$. Then, the volume element invariant under the general coordinate transformation is given by

$$d^4\tilde{x} = \sqrt{-g} d^4x. \quad (3.7)$$

In the following, we introduce scalar, vector, and tensor quantities according to properties under the coordinate transformation $x^\mu \rightarrow \tilde{x}^\mu$. First of all, a scalar field ϕ is a coordinate-independent quantity defined at each spacetime point, such that

$$\phi(\tilde{x}) = \phi(x). \quad (3.8)$$

A contravariant vector A^μ is a quantity that transforms in the same way as dx^μ in Eq. (3.2), such that

$$\tilde{A}^\alpha = \frac{\partial \tilde{x}^\alpha}{\partial x^\mu} A^\mu. \quad (3.9)$$

A covariant vector B_μ is a quantity transforming in the following manner:

$$\tilde{B}_\alpha = \frac{\partial x^\mu}{\partial \tilde{x}^\alpha} B_\mu. \quad (3.10)$$

Taking the derivative of Eq. (3.8) with respect to $\tilde{x}^\alpha$, we find that the quantity $\partial\phi/\partial x^\mu$ corresponds to the covariant vector.

A mixed m -rank contravariant and n -rank covariant tensor $T^{\mu_1\mu_2\cdots\mu_m}_{\nu_1\nu_2\cdots\nu_n}$ obeys the transformation law

$$\tilde{T}^{\alpha_1\alpha_2\cdots\alpha_m}_{\beta_1\beta_2\cdots\beta_n} = \frac{\partial \tilde{x}^{\alpha_1}}{\partial x^{\mu_1}} \frac{\partial \tilde{x}^{\alpha_2}}{\partial x^{\mu_2}} \cdots \frac{\partial \tilde{x}^{\alpha_m}}{\partial x^{\mu_m}} \frac{\partial x^{\nu_1}}{\partial \tilde{x}^{\beta_1}} \frac{\partial x^{\nu_2}}{\partial \tilde{x}^{\beta_2}} \cdots \frac{\partial x^{\nu_n}}{\partial \tilde{x}^{\beta_n}} T^{\mu_1\mu_2\cdots\mu_m}_{\nu_1\nu_2\cdots\nu_n}. \quad (3.11)$$

For example, the two-rank contravariant metric tensor $g^{\mu\nu}$ and the two-rank covariant metric tensor $g_{\mu\nu}$ satisfy

$$\tilde{g}^{\alpha\beta} = \frac{\partial \tilde{x}^\alpha}{\partial x^\mu} \frac{\partial \tilde{x}^\beta}{\partial x^\nu} g^{\mu\nu}, \quad (3.12)$$

$$\tilde{g}_{\alpha\beta} = \frac{\partial x^\mu}{\partial \tilde{x}^\alpha} \frac{\partial x^\nu}{\partial \tilde{x}^\beta} g_{\mu\nu}, \quad (3.13)$$

respectively. In fact, the latter relation is consistent with Eq. (3.3).

From the contravariant vector A^ν , the covariant vector A_μ can be constructed as

$$A_\mu = g_{\mu\nu} A^\nu. \quad (3.14)$$

On using Eqs. (3.9) and (3.13), it follows that the vector field A_μ introduced by Eq. (3.14) obeys the transformation law (3.10). Similarly, we can construct the contravariant vector B^μ from the covariant vector B_λ , as

$$B^\mu = g^{\mu\lambda} B_\lambda. \quad (3.15)$$

There is the relation between the covariant and contravariant metric tensors:

$$g_{\mu\nu} g^{\nu\lambda} = \delta_\mu^\lambda, \quad (3.16)$$

where δ_μ^λ is the Kronecker delta, i.e., $\delta_\mu^\lambda = 1$ for $\lambda = \mu$ and $\delta_\mu^\lambda = 0$ for $\lambda \neq \mu$. Taking the product of A_μ and B^μ and using Eq. (3.16), we obtain the relation $A_\mu B^\mu = A^\lambda B_\lambda$. This corresponds to the scalar product $g_{\mu\nu} A^\mu B^\nu$ satisfying the property (3.8).

3.2. Curvatures

Let us consider a covariant vector $V_\nu(x)$ at a point A (labelled by the coordinate x) in a curved spacetime. Suppose that this vector field moves under an infinitesimal parallel transport to another point B (labelled by the coordinate $x + \Delta x$). On the curved background, the shifted vector field $\tilde{V}_\nu(x + \Delta x)$ is generally different from the original vector field $V_\nu(x)$. We quantify this difference according to the relation

$$\tilde{V}_\nu(x + \Delta x) - V_\nu(x) = \Gamma_{\nu\lambda}^\mu V_\mu \Delta x^\lambda, \quad (3.17)$$

where $\Gamma_{\nu\lambda}^\mu$ is called a Christoffel symbol or an Affine connection.

The Christoffel symbol can be expressed in terms of the metric tensor $g_{\mu\nu}$ and its derivatives with respect to the coordinate x^μ . In doing so, we use the fact that the length of a four-dimensional vector field is invariant under the parallel translation. In addition, we assume that the Christoffel symbol is symmetric with respect to lower indices, as

$$\Gamma_{\nu\lambda}^\mu = \Gamma_{\lambda\nu}^\mu. \quad (3.18)$$

The condition (3.18) is attributed to the fact that a local inertial frame with vanishing Christoffel symbols can be realized.

The condition under which the length of a vector field $V_\mu(x)$ is invariant under the parallel translation can be expressed as

$$g^{\mu\nu}(x + \Delta x) \tilde{V}_\mu(x + \Delta x) \tilde{V}_\nu(x + \Delta x) = g^{\mu\nu} V_\mu(x) V_\nu(x). \quad (3.19)$$

We expand the metric $g^{\mu\nu}$ up to linear order in Δx , as

$$g^{\mu\nu}(x + \Delta x) = g^{\mu\nu}(x) + \frac{\partial g^{\mu\nu}}{\partial x^\lambda} \Delta x^\lambda + \mathcal{O}((\Delta x)^2), \quad (3.20)$$

and apply Eq. (3.17) to the left hand side of Eq. (3.19). To satisfy the condition (3.19) for any values of V_μ and Δx , we require that

$$\frac{\partial g^{\mu\nu}}{\partial x^\lambda} + g^{\rho\nu} \Gamma_{\rho\lambda}^\mu + g^{\mu\rho} \Gamma_{\rho\lambda}^\nu = 0. \quad (3.21)$$

From Eq. (3.16) there is the relation $(g_{\mu\nu} + \delta g_{\mu\nu})(g^{\nu\lambda} + \delta g^{\nu\lambda}) = \delta_\mu^\lambda$, where $\delta g_{\mu\nu}$ is the shift of the metric induced by Eq. (3.20). Up to linear order in $\delta g_{\mu\nu}$, we have that $g_{\mu\nu} \delta g^{\nu\lambda} = -g^{\nu\lambda} \delta g_{\mu\nu}$. Multiplying this relation by $g^{\rho\mu}$, we obtain $\delta g^{\rho\lambda} = -g^{\rho\mu} g^{\lambda\nu} \delta g_{\mu\nu}$. This gives the relation

$$\frac{\partial g^{\mu\nu}}{\partial x^\lambda} = -g^{\mu\alpha} g^{\nu\beta} \frac{\partial g_{\alpha\beta}}{\partial x^\lambda}. \quad (3.22)$$

Since the second and third terms on the left hand side of Eq. (3.21) are equivalent to $g^{\nu\beta}g^{\mu\alpha}g_{\alpha\gamma}\Gamma_{\beta\lambda}^\gamma$ and $g^{\mu\alpha}g^{\nu\beta}g_{\beta\gamma}\Gamma_{\alpha\lambda}^\gamma$, respectively, it follows that

$$\frac{\partial g_{\alpha\beta}}{\partial x^\lambda} = g_{\alpha\gamma}\Gamma_{\beta\lambda}^\gamma + g_{\beta\gamma}\Gamma_{\alpha\lambda}^\gamma. \quad (3.23)$$

From this, we can show that the Christoffel symbol is expressed in the form

$$\Gamma_{\nu\lambda}^\mu = \frac{1}{2}g^{\mu\rho}(g_{\rho\nu,\lambda} + g_{\rho\lambda,\nu} - g_{\nu\lambda,\rho}), \quad (3.24)$$

where $g_{\rho\nu,\lambda} \equiv \partial g_{\rho\nu}/\partial x^\lambda$. On the Minkowski background ($g_{\mu\nu} = \eta_{\mu\nu}$), all the components of Christoffel symbols vanish, but this is not the case for $\Gamma_{\nu\lambda}^\mu$ in the curved spacetime.

If we consider a set of basis vectors $\mathbf{e}_\mu(x)$ in the tangent space at a spacetime point x , the meaning of the Christoffel symbol becomes clear [3]. For two near points P and Q characterized by coordinates x^μ and $x^\mu + dx^\mu$, their infinitesimal distance is given by $d\mathbf{s} = \mathbf{e}_\mu(x)dx^\mu$. Comparing the squared of the four-dimensional distance $ds^2 = d\mathbf{s} \cdot d\mathbf{s} = \mathbf{e}_\mu(x) \cdot \mathbf{e}_\nu(x)dx^\mu dx^\nu$ with Eq. (3.1), we find

$$g_{\mu\nu}(x) = \mathbf{e}_\mu(x) \cdot \mathbf{e}_\nu(x). \quad (3.25)$$

The Christoffel symbol $\Gamma_{\nu\lambda}^\mu$ is related to the derivative of basis vectors $\mathbf{e}_\mu(x)$, as

$$\frac{\partial \mathbf{e}_\nu}{\partial x^\lambda} = \Gamma_{\nu\lambda}^\mu \mathbf{e}_\mu. \quad (3.26)$$

We can confirm that this definition is consistent with Eqs. (3.23) and (3.24). On using Eqs. (3.25) and (3.26), for example, the left hand side of Eq. (3.23) reduces to

$$\begin{aligned} \frac{\partial g_{\alpha\beta}}{\partial x^\lambda} &= \mathbf{e}_\alpha \cdot \mathbf{e}_{\beta,\lambda} + \mathbf{e}_{\alpha,\lambda} \cdot \mathbf{e}_\beta \\ &= (\mathbf{e}_\alpha \cdot \mathbf{e}_\gamma)\Gamma_{\beta\lambda}^\gamma + (\mathbf{e}_\beta \cdot \mathbf{e}_\gamma)\Gamma_{\alpha\lambda}^\gamma \\ &= g_{\alpha\gamma}\Gamma_{\beta\lambda}^\gamma + g_{\beta\gamma}\Gamma_{\alpha\lambda}^\gamma, \end{aligned} \quad (3.27)$$

which is equivalent to the right hand side of Eq. (3.23). The relation (3.26) shows that the Christoffel symbol characterizes the change of tangent vector $\mathbf{e}_\nu(x)$ at each spacetime point x .

On curved backgrounds, the parallel-transported vector $\tilde{V}_\nu(x + \Delta x)$ at the point B is not identical to the vector $V_\nu(x + \Delta x)$ at the same point. To quantify this difference, we define a covariant derivative of the covariant vector field $V_\nu(x)$, as

$$\begin{aligned} V_{\nu;\lambda}(x) = \nabla_\lambda V_\nu &\equiv \lim_{\Delta x^\lambda \rightarrow 0} \frac{V_\nu(x + \Delta x) - \tilde{V}_\nu(x + \Delta x)}{\Delta x^\lambda} \\ &= V_{\nu,\lambda}(x) - \Gamma_{\nu\lambda}^\mu(x)V_\mu(x), \end{aligned} \quad (3.28)$$

where we used Eq. (3.17) in the second line. The scalar product $A^\mu(x)B_\mu(x)$ of contravariant vector $A^\mu(x)$ and covariant vector $B_\mu(x)$ is invariant under the parallel

translation, such that

$$\tilde{A}^\mu(x + \Delta x)\tilde{B}_\mu(x + \Delta x) = A^\mu(x)B_\mu(x). \quad (3.29)$$

We express the shift of the vector field A^μ as $\tilde{A}^\mu(x + \Delta x) = A^\mu(x) + \delta A^\mu$ and then substitute this relation and $\tilde{B}_\mu(x + \Delta x) = B_\mu(x) + \Gamma_{\mu\lambda}^\nu B_\nu \Delta x^\lambda$ into Eq. (3.29). Then, we obtain $B_\mu \delta A^\mu = -B_\nu A^\mu \Gamma_{\mu\lambda}^\nu \Delta x^\lambda = -B_\mu A^\nu \Gamma_{\nu\lambda}^\mu \Delta x^\lambda$ at linear order in δA^μ and Δx^λ . This gives $\delta A^\mu = -\Gamma_{\nu\lambda}^\mu A^\nu \Delta x^\lambda$ and hence

$$\tilde{A}^\mu(x + \Delta x) = A^\mu(x) - \Gamma_{\nu\lambda}^\mu A^\nu \Delta x^\lambda. \quad (3.30)$$

On using this relation, the covariant derivative of the contravariant vector field $A^\mu(x)$ reads

$$\begin{aligned} \nabla_\lambda A^\mu &= A^\mu{}_{;\lambda}(x) \equiv \lim_{\Delta x^\lambda \rightarrow 0} \frac{A^\mu(x + \Delta x) - \tilde{A}^\mu(x + \Delta x)}{\Delta x^\lambda} \\ &= A^\mu{}_{;\lambda}(x) + \Gamma_{\nu\lambda}^\mu A^\nu(x). \end{aligned} \quad (3.31)$$

The covariant vector of mixed second rank tensor $T^\mu{}_\nu = A^\mu B_\nu$, which is the product of contravariant vector A^μ and covariant vector B_ν , is given by

$$\nabla_\lambda T^\mu{}_\nu = T^\mu{}_{\nu;\lambda} + \Gamma_{\rho\lambda}^\mu T^\rho{}_\nu - \Gamma_{\nu\lambda}^\rho T^\mu{}_\rho. \quad (3.32)$$

The covariant derivative of a tensor with rank higher than two also has a similar property to Eq. (3.32), i.e., plus and minus signs arise in front of Christoffel symbols for the contravariant and covariant parts of tensor respectively. From Eq. (3.32), we find that the metric tensor obeys $\nabla_\lambda g_{\mu\nu} = g_{\mu\nu;\lambda} - \Gamma_{\mu\lambda}^\rho g_{\nu\rho} - \Gamma_{\nu\lambda}^\rho g_{\mu\rho}$. On using Eq. (3.23), it follows that

$$\nabla_\lambda g_{\mu\nu} = 0. \quad (3.33)$$

This means that, after the parallel translation, the metric tensor $g_{\mu\nu}$ has the same value at the shifted point.

On the curved spacetime, the vector field after parallel translations is different depending on chosen routes. Let us consider an infinitesimal area $\Delta x^\lambda \Delta x^\rho$ surrounded by the four points O: (x^λ, x^ρ) , P₁: $(x^\lambda + \Delta x^\lambda, x^\rho)$, Q: $(x^\lambda + \Delta x^\lambda, x^\rho + \Delta x^\rho)$, and P₂: $(x^\lambda, x^\rho + \Delta x^\rho)$; see Fig. 3.1. Under the parallel translation of a contravariant vector field A^μ from O to P₁, we have

$$\tilde{A}^\mu(P_1) = A^\mu(O) - \Gamma_{\nu\lambda}^\mu(O) A^\nu(O) \Delta x^\lambda. \quad (3.34)$$

Similarly, the parallel translation from P₁ to Q gives

$$\tilde{A}^\mu(Q) = \tilde{A}^\mu(P_1) - \Gamma_{\nu\rho}^\mu(P_1) \tilde{A}^\nu(P_1) \Delta x^\rho. \quad (3.35)$$

At linear order in Δx^λ , the difference between $\Gamma_{\nu\rho}^\mu(O)$ and $\Gamma_{\nu\rho}^\mu(P_1)$ is given by

$$\Gamma_{\nu\rho}^\mu(P_1) = \Gamma_{\nu\rho}^\mu(O) + \Gamma_{\nu\rho,\lambda}^\mu(O) \Delta x^\lambda. \quad (3.36)$$

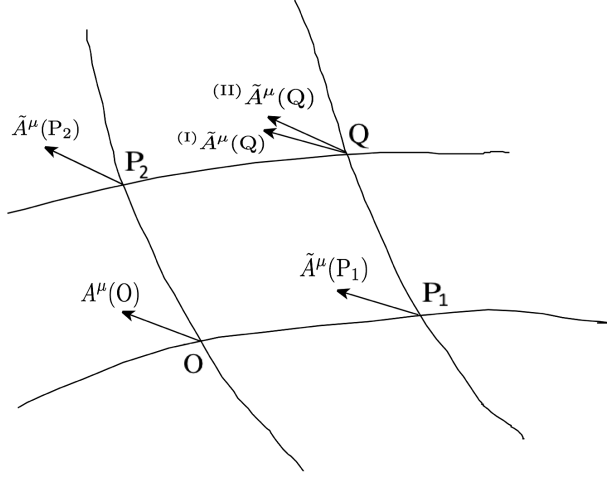


Fig. 3.1. Parallel translations of a vector field A^μ in an infinitesimal area surrounded by the four points O, P_1, Q, P_2 . There are two routes from the point O to Q : (I) $O \rightarrow P_1 \rightarrow Q$, and (II) $O \rightarrow P_2 \rightarrow Q$. The two parallel-translated vectors at the point Q along the routes (I) and (II) are denoted as $^{(I)}\tilde{A}^\mu(Q)$ and $^{(II)}\tilde{A}^\mu(Q)$ in the figure, respectively.

Then, after the parallel translation by the route $O \rightarrow P_1 \rightarrow Q$ (labeled by I), the difference $^{(I)}\Delta\tilde{A}^\mu = \tilde{A}^\mu(Q) - A^\mu(O)$ reads

$$^{(I)}\Delta\tilde{A}^\mu = -\Gamma_{\nu\lambda}^\mu A^\nu \Delta x^\lambda - \Gamma_{\nu\rho}^\mu A^\nu \Delta x^\rho - \left(\Gamma_{\nu\rho,\lambda}^\mu - \Gamma_{\alpha\rho}^\mu \Gamma_{\nu\lambda}^\alpha \right) A^\nu \Delta x^\lambda \Delta x^\rho. \quad (3.37)$$

Similarly, the change of A^μ after the parallel translation by the route $O \rightarrow P_2 \rightarrow Q$ (labeled by II) can be derived by exchanging the labels λ and ρ in Eq. (3.37), i.e.,

$$^{(II)}\Delta\tilde{A}^\mu = -\Gamma_{\nu\rho}^\mu A^\nu \Delta x^\rho - \Gamma_{\nu\lambda}^\mu A^\nu \Delta x^\lambda - \left(\Gamma_{\nu\lambda,\rho}^\mu - \Gamma_{\alpha\lambda}^\mu \Gamma_{\nu\rho}^\alpha \right) A^\nu \Delta x^\rho \Delta x^\lambda. \quad (3.38)$$

Then, the difference between $^{(I)}\Delta\tilde{A}^\mu$ and $^{(II)}\Delta\tilde{A}^\mu$ is given by

$$\begin{aligned} \Delta A^\mu &\equiv ^{(II)}\Delta\tilde{A}^\mu - ^{(I)}\Delta\tilde{A}^\mu \\ &= \left(\Gamma_{\nu\rho,\lambda}^\mu - \Gamma_{\nu\lambda,\rho}^\mu + \Gamma_{\alpha\lambda}^\mu \Gamma_{\nu\rho}^\alpha - \Gamma_{\alpha\rho}^\mu \Gamma_{\nu\lambda}^\alpha \right) A^\nu \Delta x^\lambda \Delta x^\rho. \end{aligned} \quad (3.39)$$

We write this difference in the form

$$\Delta A^\mu = R^\mu{}_{\nu\lambda\rho} A^\nu \Delta x^\lambda \Delta x^\rho, \quad (3.40)$$

where $R^\mu{}_{\nu\lambda\rho}$ is called the Riemann tensor defined by

$$R^\mu{}_{\nu\lambda\rho} = \Gamma_{\nu\rho,\lambda}^\mu - \Gamma_{\nu\lambda,\rho}^\mu + \Gamma_{\alpha\lambda}^\mu \Gamma_{\nu\rho}^\alpha - \Gamma_{\alpha\rho}^\mu \Gamma_{\nu\lambda}^\alpha. \quad (3.41)$$

Hence the Riemann tensor characterizes the difference between two parallel transported vectors $^{(I)}\tilde{A}^\mu(Q)$ and $^{(II)}\tilde{A}^\mu(Q)$ on curved backgrounds.

On using the definition (3.24) of the Christoffel symbol, the Riemann tensor with four lower indices can be expressed as

$$\begin{aligned} R_{\sigma\nu\lambda\rho} &\equiv g_{\sigma\mu} R^{\mu}{}_{\nu\lambda\rho} \\ &= \frac{1}{2} (g_{\sigma\rho, \nu\lambda} + g_{\nu\lambda, \sigma\rho} - g_{\nu\rho, \sigma\lambda} - g_{\sigma\lambda, \nu\rho}) + g_{\alpha\beta} \left(\Gamma_{\sigma\rho}^{\alpha} \Gamma_{\nu\lambda}^{\beta} - \Gamma_{\sigma\lambda}^{\alpha} \Gamma_{\nu\rho}^{\beta} \right). \end{aligned} \quad (3.42)$$

From this relation, it follows that

$$R_{\sigma\nu\lambda\rho} = -R_{\nu\sigma\lambda\rho} = -R_{\sigma\nu\rho\lambda}, \quad (3.43)$$

$$R_{\sigma\nu\lambda\rho} = R_{\lambda\rho\sigma\nu}, \quad (3.44)$$

$$R_{\sigma\nu\lambda\rho} + R_{\sigma\lambda\rho\nu} + R_{\sigma\rho\nu\lambda} = 0. \quad (3.45)$$

The quantity $[\nabla_{\mu}, \nabla_{\nu}]A_{\rho}$, where $[\nabla_{\mu}, \nabla_{\nu}] \equiv \nabla_{\mu}\nabla_{\nu} - \nabla_{\nu}\nabla_{\mu}$ and A_{ρ} is an arbitrary vector field, can be expressed in terms of the Riemann tensor. On using

$$\nabla_{\mu}\nabla_{\nu}A_{\rho} = \partial_{\mu}(\nabla_{\nu}A_{\rho}) - \Gamma_{\rho\mu}^{\sigma}\nabla_{\nu}A_{\sigma} - \Gamma_{\nu\mu}^{\sigma}\nabla_{\sigma}A_{\rho}, \quad (3.46)$$

with $\nabla_{\nu}A_{\rho} = A_{\rho, \nu} - \Gamma_{\nu\rho}^{\sigma}A_{\sigma}$, we find

$$[\nabla_{\mu}, \nabla_{\nu}]A_{\rho} = R^{\sigma}{}_{\rho\nu\mu}A_{\sigma}. \quad (3.47)$$

Similarly, we obtain the following relation

$$[\nabla_{\mu}, \nabla_{\nu}]\nabla_{\lambda}A_{\rho} = R^{\sigma}{}_{\lambda\nu\mu}\nabla_{\sigma}A_{\rho} + R^{\sigma}{}_{\rho\nu\mu}\nabla_{\lambda}A_{\sigma}. \quad (3.48)$$

Due to the anti-symmetric property of the operator $[\nabla_{\mu}, \nabla_{\nu}]$, we have

$$([\nabla_{\lambda}, [\nabla_{\mu}, \nabla_{\nu}]] + [\nabla_{\mu}, [\nabla_{\nu}, \nabla_{\lambda}]] + [\nabla_{\nu}, [\nabla_{\lambda}, \nabla_{\mu}]])A_{\rho} = 0. \quad (3.49)$$

Substituting the relations (3.47) and (3.48) into Eq. (3.49) and using Eq. (3.45), it follows that

$$(\nabla_{\lambda}R^{\sigma}{}_{\rho\nu\mu} + \nabla_{\mu}R^{\sigma}{}_{\rho\lambda\nu} + \nabla_{\nu}R^{\sigma}{}_{\rho\mu\lambda})A_{\sigma} = 0. \quad (3.50)$$

Since this holds for any vector A_{σ} , we obtain

$$\nabla_{\lambda}R^{\sigma}{}_{\rho\nu\mu} + \nabla_{\mu}R^{\sigma}{}_{\rho\lambda\nu} + \nabla_{\nu}R^{\sigma}{}_{\rho\mu\lambda} = 0, \quad (3.51)$$

which is called the Bianchi identity.

We define the Ricci tensor $R_{\nu\rho}$ and the Ricci scalar R , as

$$R_{\nu\rho} \equiv R^{\mu}{}_{\nu\mu\rho} = \Gamma_{\nu\rho, \mu}^{\mu} - \Gamma_{\nu\mu, \rho}^{\mu} + \Gamma_{\alpha\mu}^{\mu} \Gamma_{\nu\rho}^{\alpha} - \Gamma_{\alpha\rho}^{\mu} \Gamma_{\nu\mu}^{\alpha}, \quad (3.52)$$

$$R \equiv g^{\nu\rho}R_{\nu\rho}, \quad (3.53)$$

where the Ricci tensor satisfies the symmetric relation $R_{\nu\rho} = R_{\rho\nu}$. Setting $\sigma = \nu$ in Eq. (3.51) and using Eq. (3.43), we find

$$\nabla_\lambda R_{\rho\mu} - \nabla_\mu R_{\rho\lambda} + \nabla_\nu R^\nu_{\rho\mu\lambda} = 0. \quad (3.54)$$

Multiplying Eq. (3.54) by $g^{\rho\lambda}$ on account of the property (3.33), we obtain

$$2\nabla_\lambda R^\lambda_\mu - \nabla_\mu R = 0. \quad (3.55)$$

This can be expressed as

$$\nabla_\lambda G^\lambda_\mu = 0, \quad (3.56)$$

where G^λ_μ is called the Einstein tensor defined by

$$G^\lambda_\mu \equiv R^\lambda_\mu - \frac{1}{2}\delta^\lambda_\mu R. \quad (3.57)$$

Multiplying Eq. (3.57) by $g_{\lambda\nu}$ leads to the two-rank covariant Einstein tensor:

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R. \quad (3.58)$$

The relation (3.56) following from the Bianchi identity can also be written in the form

$$\nabla_\mu G^{\mu\nu} = 0, \quad (3.59)$$

where $G^{\mu\nu} = R^{\mu\nu} - (1/2)g^{\mu\nu}R$ is the two-rank contravariant Einstein tensor. This property plays an important role in the derivation of the Einstein equation in Sec. 3.3.

3.3. Einstein equations

So far, we have used geometric quantities to describe the curvature of spacetime qualitatively. Since the existence of matter and energy affects the curvature of spacetime, Einstein tried to relate geometric tensors with those in the matter sector. The matter distribution can be described by a so-called energy-momentum tensor. The theory of gravity should also be constructed in such a way that Newton's laws of gravitation are recovered in the weak field limit.

In Newton gravity, the gravitational potential ϕ at a point $\mathbf{x} = (x, y, z)$ induced by matter with a density distribution $\rho(\mathbf{x}')$ is given by

$$\phi(\mathbf{x}) = -G \int d^3x' \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}, \quad (3.60)$$

where G is the gravitational constant. The gravitational potential obeys the Poisson equation

$$\nabla^2 \phi = 4\pi G \rho, \quad (3.61)$$

where $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ is the three-dimensional Laplacian.

A freely falling particle follows a path that minimizes the proper interval ds on curved backgrounds. This path is called a geodesic, which corresponds to a particle trajectory moving along tangent vectors at each curved spacetime point x^μ . We characterize the geodesic as a curve $x^\mu(\lambda)$ parameterized by a parameter λ (which is called an Affine parameter). Let us consider a contravariant vector V^μ at each point x^μ . On using basis vectors e_μ in the tangent space (which was introduced in Sec. 3.2), we introduce a local vector field

$$V(\lambda) = V^\mu(\lambda) e_\mu(\lambda), \quad (3.62)$$

at each point $x^\mu(\lambda)$. The geodesic is characterized by a trajectory along which the local tangent vector (3.62) is the same at all points along the curve, such that

$$\frac{dV}{d\lambda} = 0, \quad (3.63)$$

which translates to

$$\frac{dV}{d\lambda} = \frac{dV^\mu}{d\lambda} e_\mu + V^\mu \frac{\partial e_\mu}{\partial x^\nu} \frac{dx^\nu}{d\lambda} = 0. \quad (3.64)$$

Substituting Eq. (3.26), i.e., $\partial e_\mu/\partial x^\nu = \Gamma_{\mu\nu}^\rho e_\rho$, into Eq. (3.64) and changing dummy indices μ, ν, ρ in the second term of Eq. (3.64) to α, β, μ respectively, it follows that

$$\frac{dV}{d\lambda} = \left(\frac{dV^\mu}{d\lambda} + \Gamma_{\alpha\beta}^\mu V^\alpha \frac{dx^\beta}{d\lambda} \right) e_\mu = 0. \quad (3.65)$$

Since the components of the tangent vector are given by $V^\mu = dx^\mu/d\lambda$, the requirement that Eq. (3.65) holds for any e_μ leads to the geodesic equation

$$\frac{d^2 x^\mu}{d\lambda^2} + \Gamma_{\alpha\beta}^\mu \frac{dx^\alpha}{d\lambda} \frac{dx^\beta}{d\lambda} = 0. \quad (3.66)$$

This equation can be applied to both massless and massive particles. The second term on the left hand side of Eq. (3.66) can be regarded as a gravitational force induced by the curved geometric structure with non-vanishing Christoffel symbols.

For a freely falling particle with a non-zero mass m , the four velocity is given by $u^\mu = dx^\mu/d\tau$, where τ is a proper time related to the line element ds as $ds^2 = -c^2 d\tau^2 = dx^\mu dx_\mu$. From this latter relation we obtain $u^\mu u_\mu = -c^2$, so the four velocity is constant in a local inertial frame. In this case, the affine parameter λ can be identified as the proper time τ , so that the tangent vector $V^\mu = dx^\mu/d\lambda$

is equivalent to the four velocity $u^\mu = dx^\mu/d\tau$. Then, for a massive particle, the geodesic equation (3.66) reads

$$\frac{d^2 x^\mu}{d\tau^2} + \Gamma_{\alpha\beta}^\mu \frac{dx^\alpha}{d\tau} \frac{dx^\beta}{d\tau} = 0. \quad (3.67)$$

Let us take the limit of weak gravity for the geodesic equation (3.67). In doing so, we assume the following conditions: (i) $g_{\mu\nu}$ is close to the Minkowski value $\eta_{\mu\nu}$ with a small perturbation $h_{\mu\nu}$, i.e., $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$ with $|h_{\mu\nu}| \ll 1$, (ii) $h_{\mu\nu}$ does not depend on the time t , (iii) $g_{0i} = g_{i0} = 0$, and (iv) the spatial velocity $u^i = dx^i/d\tau$ of the freely falling particle is much smaller than the speed of light c . The gravitational field is stationary and static under the assumptions (ii) and (iii).

Under the assumptions (i) and (iv), we neglect second-order terms in $h_{\mu\nu}$ and u^i . Then, the Christoffel symbol reads

$$\Gamma_{\nu\lambda}^\mu \simeq \frac{1}{2} \eta^{\mu\rho} (h_{\rho\nu,\lambda} + h_{\rho\lambda,\nu} - h_{\nu\lambda,\rho}), \quad (3.68)$$

which is first order in $h_{\mu\nu}$. Since there is the relation $-c^2 dt^2/d\tau^2 + \sum_{i=1}^3 (u^i)^2 = -c^2$, it follows that $d\tau \simeq dt$ under the above approximation scheme. From the geodesic equation (3.67), the spatial vector x^i obeys the differential equation

$$\ddot{x}^i \simeq -\Gamma_{\alpha\beta}^i \dot{x}^\alpha \dot{x}^\beta \simeq -c^2 \Gamma_{00}^i, \quad (3.69)$$

where a dot represents a derivative with respect to t . In the second approximate equality of Eq. (3.69), we picked up contributions up to first order in $h_{\mu\nu}$. From Eq. (3.68), we have

$$\Gamma_{00}^i \simeq -\frac{1}{2} h_{00,i} \simeq -\frac{1}{2} \partial^i h_{00}, \quad (3.70)$$

so that Eq. (3.69) reduces to

$$\ddot{x}^i = \frac{c^2}{2} \partial^i h_{00}. \quad (3.71)$$

In Newton gravity, the equation of motion for the freely falling particle is given by

$$\ddot{x}^i = -\partial^i \phi, \quad (3.72)$$

where ϕ is the gravitational potential. From Eqs. (3.71) and (3.72) we obtain the correspondence

$$\phi = -\frac{c^2}{2} h_{00}. \quad (3.73)$$

On using the correspondence, the Poisson equation (3.61) can be written as

$$\nabla^2 h_{00} = -\frac{8\pi G}{c^2} \rho. \quad (3.74)$$

This shows that the metric h_{00} is directly related to the density ρ of non-relativistic matter. The Einstein equations, which relate the spacetime geometry with the matter distribution, should recover Eq. (3.74) in the limit of weak gravity. Since geometric tensor quantities were already introduced in Sec. 3.2, we now discuss tensor quantities associated with the matter distribution.

Let us consider a general fluid distributed in the four-dimensional spacetime. We begin with an infinitesimal three-dimensional surface with a constant coordinate value x^ν . For the constant temporal coordinate x^0 , the three-dimensional surface orthogonal to x^0 corresponds to a three-dimensional spatial volume. We define an energy-momentum tensor $T^{\mu\nu}$ as the four momentum $P^\mu = mu^\mu$ passing through the three-dimensional surface per unit volume (which is called a flux).

The component T^{00} is attributed to the energy per volume (energy density) passing through a three-dimensional spatial volume with constant x^0 . The temporal-spatial component T^{0i} refers to the energy flux that passes through two-dimensional unit area orthogonal to the coordinate x^i per unit time. The spatial-temporal component T^{i0} corresponds to the i th momentum P^i passing through the three-dimensional spatial unit volume. The spatial-spatial component T^{ij} refers to the i th momentum P^i passing through a two-dimensional unit area orthogonal to the coordinate x^j per unit time. Since the momentum P^i per unit time exerts a force F^i on the two-dimensional area orthogonal to x^j , the component T^{ij} is called a stress tensor. The energy-momentum tensor satisfies the symmetric relation $T^{\mu\nu} = T^{\nu\mu}$.

In the fluid rest frame, the component T^{00} is directly related to the fluid energy density ρc^2 . In the absence of heat conductivity and viscosity, there are no off-diagonal components, i.e., $T^{0i} = T^{i0} = 0$ and $T^{ij} = 0$ ($i \neq j$). In this case the fluid is called a perfect fluid, which has an isotropic pressure P in each spatial dimension. Thus, in the rest frame, the energy-momentum tensor of the perfect fluid has only diagonal components, as

$$T^\mu{}_\lambda = \text{diag}(-\rho c^2, P, P, P), \quad (3.75)$$

which gives $T^{00} = \rho c^2$ and $T^{11} = T^{22} = T^{33} = P$ in the Minkowski spacetime.

In terms of the four velocity u^μ of the perfect fluid, its energy-momentum tensor is restricted to the form $T^\mu{}_\lambda = \alpha_1 u^\mu u_\lambda + \alpha_2 \delta^\mu_\lambda$. To recover Eq. (3.75) in the rest frame with $u^\mu = (c, 0, 0, 0)$, the coefficients α_1 and α_2 are fixed to be $\alpha = \rho + P/c^2$ and $\alpha_2 = P$. Thus the energy-momentum tensor is given by

$$T^\mu{}_\lambda = \left(\rho + \frac{P}{c^2} \right) u^\mu u_\lambda + P \delta^\mu_\lambda. \quad (3.76)$$

Multiplying Eq. (3.76) by $g^{\nu\lambda}$, it follows that

$$T^{\mu\nu} = \left(\rho + \frac{P}{c^2} \right) u^\mu u^\nu + P g^{\mu\nu}. \quad (3.77)$$

In the Minkowski spacetime, the conservation of energy and momentum corresponds to the continuity equation $\partial_\mu T^{\mu\nu} = 0$. In the curved spacetime, the partial derivative needs to be replaced with the covariant derivative, so the continuity equation is modified to

$$\nabla_\mu T^{\mu\nu} = 0. \quad (3.78)$$

We recall that the Einstein tensor $G^{\mu\nu}$ satisfies the relation (3.59) analogous to Eq. (3.78). Hence the spacetime geometry (characterized by $G_{\mu\nu} = R_{\mu\nu} - (1/2)g_{\mu\nu}R$) can be related with the matter sector (characterized by $T_{\mu\nu}$) in the form

$$G_{\mu\nu} = \kappa^2 T_{\mu\nu}. \quad (3.79)$$

The constant κ^2 is determined by requiring that Newton gravity is recovered under the weak field approximation. Multiplying Eq. (3.79) by $g^{\mu\nu}$ and taking the trace of it, we obtain

$$R = -\kappa^2 T, \quad (3.80)$$

where $T \equiv g^{\mu\nu}T_{\mu\nu} = T^\mu_\mu$. Substituting this relation into Eq. (3.79), the Ricci tensor can be expressed as

$$R_{\mu\nu} = \kappa^2 \left(T_{\mu\nu} - \frac{1}{2}g_{\mu\nu}T \right). \quad (3.81)$$

Under the approximation of weak gravity, it follows that

$$R_{00} \simeq \Gamma_{00,i}^i \simeq -\frac{1}{2}\nabla^2 h_{00}. \quad (3.82)$$

For non-relativistic matter, the pressure term P/c^2 can be negligible relative to ρ in Eq. (3.76), so that $T = -\rho c^2 + 3P \simeq -\rho c^2$ and $T_{00} \simeq \rho c^2$. Since the (00) component on the right hand side of Eq. (3.81) is approximately given by

$$\kappa^2 \left(T_{00} - \frac{1}{2}g_{00}T \right) \simeq \frac{1}{2}\kappa^2 \rho c^2, \quad (3.83)$$

we obtain the following relation

$$\nabla^2 h_{00} \simeq -\kappa^2 \rho c^2. \quad (3.84)$$

Comparing this with the Poisson equation (3.74), the coefficient κ^2 is fixed as $\kappa^2 = 8\pi G/c^4$. Then, the field equation of motion (3.79) becomes

$$G_{\mu\nu} = \frac{8\pi G}{c^4} T_{\mu\nu}, \quad (3.85)$$

which was derived by Einstein in 1915. The Einstein equation (3.85) is valid not only in the case of weak gravity but also on strong gravitational backgrounds. It can

be applied to a wide range of gravitational phenomena, e.g., expanding Universe, black holes, and gravitational waves.

Since the metric tensor obeys the relation (3.33), we are free to add a term $\Lambda g_{\mu\nu}$, where Λ is a constant. In this case, the Einstein equation (3.85) is modified to

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = \frac{8\pi G}{c^4} T_{\mu\nu}. \quad (3.86)$$

The term Λ is dubbed a cosmological constant, which was first introduced by Einstein to realize a static Universe. In the presence of the cosmological constant the Poisson equation (3.84) is subject to change, so such a new term needs to be small for the consistency with local gravity experiments in the solar system. As we will see later in Sec. 4.4, the cosmological constant can drive the cosmic acceleration, which is one of the main topics in this book.

3.4. Variational principle

The Einstein equation (3.86) can also be derived by using a variational principle of least action. Let us consider the following action:

$$S = \frac{c^3}{16\pi G} \int d^4x \sqrt{-g} (R - 2\Lambda) + S_m(g_{\mu\nu}, \Psi_m), \quad (3.87)$$

where S_m is a matter action that depends on matter fields Ψ_m and the metric $g_{\mu\nu}$. In Eq. (3.87), the volume element d^4x is multiplied by the factor $\sqrt{-g}$ to ensure its invariance under a coordinate transformation; see Eq. (3.7). Varying the action (3.87) with respect to $g^{\mu\nu}$, it follows that

$$\delta S = \frac{c^3}{16\pi G} \int d^4x [\delta(\sqrt{-g})(R - 2\Lambda) + \sqrt{-g} \delta g^{\mu\nu} R_{\mu\nu} + \sqrt{-g} g^{\mu\nu} \delta R_{\mu\nu}] + \delta S_m. \quad (3.88)$$

The variation of the Ricci tensor is given by

$$\delta R_{\mu\nu} = \nabla_\lambda \delta \Gamma_{\mu\nu}^\lambda - \nabla_\nu \delta \Gamma_{\mu\rho}^\rho, \quad (3.89)$$

so that

$$g^{\mu\nu} \delta R_{\mu\nu} = \nabla_\lambda A^\lambda, \quad \text{where} \quad A^\lambda \equiv g^{\mu\nu} \delta \Gamma_{\mu\nu}^\lambda - g^{\mu\lambda} \delta \Gamma_{\mu\rho}^\rho. \quad (3.90)$$

For the computation of the quantity $\nabla_\lambda A^\lambda$, we employ the following relations

$$g_{,\lambda} = g g^{\mu\nu} g_{\mu\nu,\lambda}, \quad (3.91)$$

$$\Gamma_{\nu\mu}^\mu = \frac{1}{2} g^{\mu\rho} g_{\mu\rho,\nu} = \frac{\partial \ln(\sqrt{-g})}{\partial x^\nu}. \quad (3.92)$$

The relation (3.91) can be derived by differentiating g expressed as $g_{\mu\nu} \mathcal{G}^{(\mu\nu)}$ with respect to $g_{\mu\nu}$, where $\mathcal{G}^{(\mu\nu)}$ is a determinant of the first minor matrix (which does not depend on the element $g_{\mu\nu}$). After replacing $\mathcal{G}^{(\mu\nu)} = g g^{\mu\nu}$, it follows that

$\partial g / \partial g_{\mu\nu} = gg^{\mu\nu}$. In the second equality of Eq. (3.92) we have used Eq. (3.91). Then, the divergence of the vector A^λ can be expressed as

$$\nabla_\lambda A^\lambda = A^\lambda{}_{,\lambda} + \Gamma_{\nu\mu}^\mu A^\nu = \frac{1}{\sqrt{-g}}(\sqrt{-g}A^\lambda)_{,\lambda}, \quad (3.93)$$

so that we obtain

$$\int d^4x \sqrt{-g} g^{\mu\nu} \delta R_{\mu\nu} = \int d^4x (\sqrt{-g}A^\lambda)_{,\lambda} = \int dS_\lambda \sqrt{-g}A^\lambda, \quad (3.94)$$

where, in the second equality, we have changed it to the surface integral on account of the Gauss's theorem. Since $A^\lambda \rightarrow 0$ at the asymptotic boundary, the integral (3.94) vanishes.

The term $\delta(\sqrt{-g})$ in the action (3.88) can be written as

$$\delta(\sqrt{-g}) = -\frac{\delta g}{2\sqrt{-g}} = -\frac{1}{2}\sqrt{-g}g_{\mu\nu}\delta g^{\mu\nu}, \quad (3.95)$$

where, in the second equality, we have used the relation following from Eq. (3.91), i.e., $\delta g = gg^{\mu\nu}\delta g_{\mu\nu} = -gg_{\mu\nu}\delta g^{\mu\nu}$. Then, the action (3.88) reads

$$\delta S = \frac{c^3}{16\pi G} \int d^4x \sqrt{-g} \left(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + \Lambda g_{\mu\nu} \right) \delta g^{\mu\nu} + \delta S_m. \quad (3.96)$$

The energy-momentum tensor $T_{\mu\nu}$ is related to the variation of δS_m in terms of $g^{\mu\nu}$, as

$$\delta S_m = -\frac{1}{2c} \int d^4x \sqrt{-g} T_{\mu\nu} \delta g^{\mu\nu}, \quad (3.97)$$

so that Eq. (3.96) reduces to

$$\delta S = \frac{c^3}{16\pi G} \int d^4x \sqrt{-g} \left(G_{\mu\nu} + \Lambda g_{\mu\nu} - \frac{8\pi G}{c^4} T_{\mu\nu} \right) \delta g^{\mu\nu}. \quad (3.98)$$

From the variational principle of least action ($\delta S = 0$), we obtain the field equation

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = \frac{8\pi G}{c^4} T_{\mu\nu}, \quad (3.99)$$

which is equivalent to the Einstein equation (3.86) in the presence of Λ . The action (3.87), which contains the linear term in R , is called the Einstein-Hilbert action. The variational principle also plays a crucial role for deriving field equations in modified gravity theories, which we will discuss in the chapters after Chap. 11.

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Chapter 4

Cosmic Expansion History

To discuss the cosmic expansion history, we need to solve the Einstein equations on a time-dependent cosmological background. In doing so, we employ the cosmological principle stating that the Universe is globally homogeneous and isotropic. On small scales there are inhomogeneities responsible for the formation of compact objects, but they can be regarded as small perturbations on the homogeneous and isotropic background. In this section, we derive background equations of motion by solving Einstein equations and then study how the cosmic expansion is affected by matter species in the Universe.

4.1. The FLRW spacetime

The homogeneous and isotropic cosmological background, which is called the Friedmann-Lemaître-Robertson-Walker (FLRW) spacetime, is given by the line element

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu = -c^2 dt^2 + a^2(t) d\sigma^2, \quad (4.1)$$

where $a(t)$ is a time-dependent scale factor and $d\sigma^2$ is a time-independent three-dimensional line element. In terms of the polar coordinates (r, θ, φ) with a spatial curvature $\mathcal{K}$, we can express $d\sigma^2$ in the form

$$d\sigma^2 = \gamma_{ij} dx^i dx^j = \frac{dr^2}{1 - \mathcal{K}r^2} + r^2(d\theta^2 + \sin^2 \theta d\varphi^2). \quad (4.2)$$

The three-dimensional metric in Eq. (4.2) is given by $\gamma_{11} = (1 - \mathcal{K}r^2)^{-1}$, $\gamma_{22} = r^2$, $\gamma_{33} = r^2 \sin^2 \theta$ with the spherical coordinate $(x^1, x^2, x^3) = (r, \theta, \varphi)$.

The sign of $\mathcal{K}$ characterizes the geometry of the Universe, i.e., (1) closed Universe for $\mathcal{K} > 0$, (2) open Universe for $\mathcal{K} < 0$, and (3) flat Universe for $\mathcal{K} = 0$. For $\mathcal{K} = 0$ and $a = 1$, the line element (4.1) recovers the metric in Minkowski spacetime: $ds^2 = -c^2 dt^2 + dr^2 + r^2(d\theta^2 + \sin^2 \theta d\varphi^2)$. In the expanding Universe, the scale factor $a(t)$ is multiplied by an infinitesimal change $d\sigma$ in the spatial direction. For $\mathcal{K} = 0$

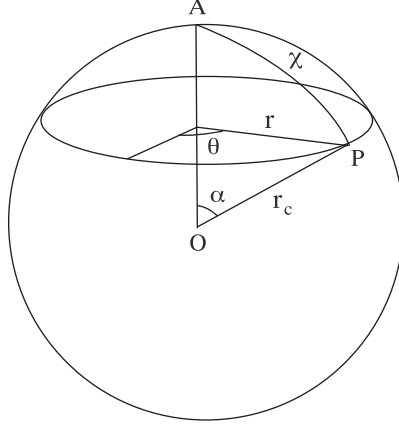


Fig. 4.1. Two-dimensional sphere embedded in a three-dimensional Euclidean space.

the change in the radial direction is given by $a(t)dr$, in which case the distance r is known as the comoving distance. For closed and open geometries, we will derive a distance χ corresponding to the comoving distance.

For $\mathcal{K} > 0$, we consider a three-dimensional spherical surface with a curvature radius r_c . In this case, the spatial curvature is given by $\mathcal{K} = 1/r_c^2$. Here, the three-dimensional spherical surface represents the one embedded in a four-dimensional Euclidean space. Under a coordinate change $r = r_c \sin(\chi/r_c)$ from r to χ , the spatial line element (4.2) is transformed to

$$d\sigma^2 = d\chi^2 + f_{\mathcal{K}}^2(\chi)(d\theta^2 + \sin^2 \theta d\varphi^2), \quad (4.3)$$

where $f_{\mathcal{K}}(\chi) = r = (1/\sqrt{\mathcal{K}}) \sin(\sqrt{\mathcal{K}}\chi)$.

Since it is difficult to illustrate the four-dimensional Euclidean space, we plot a two-dimensional spherical surface embedded in a three-dimensional Euclidean sphere (radius r_c) in Fig. 4.1. Let us consider a line between the center of sphere (O) and a point A on the surface. We denote the distance between the point A and another point P along the surface as χ . The minimal distance between the point P and the line $\overline{OA}$ is given by r . We also express the angle corresponding to the rotation along the axis $\overline{OA}$ as θ . Since the angle between the two lines $\overline{OP}$ and $\overline{OA}$ is given by $\alpha = \chi/r_c$, it follows that $r = r_c \sin(\chi/r_c)$. This is exactly the transformation used to derive Eq. (4.3).

The comoving distance corresponds to the distance χ from the point A along the two-dimensional spherical surface, so it is different from the distance r . From Fig. 4.1, the line element in the two-dimensional spherical surface is given by $d\sigma^2 = d\chi^2 + r^2 d\theta^2$. Applying this two-dimensional argument to the three-dimensional spherical surface, we obtain the spatial line element $d\sigma^2 = d\chi^2 + r^2(d\theta^2 + \sin^2 \theta d\varphi^2)$.

For $\mathcal{K} < 0$, the three-dimensional line element $d\sigma^2$ is derived by embedding a three-dimensional hyperboloid with a negative spatial curvature in the

four-dimensional Euclidean space. Setting $\mathcal{K} = -1/r_c^2$ (< 0) and performing the transformation $r = r_c \sinh(\chi/r_c)$, the metric (4.1) is transformed to

$$ds^2 = -c^2 dt^2 + a^2(t) [d\chi^2 + f_{\mathcal{K}}^2(\chi)(d\theta^2 + \sin^2 \theta d\varphi^2)], \quad (4.4)$$

where

$$f_{\mathcal{K}}(\chi) = \frac{1}{\sqrt{-\mathcal{K}}} \sinh\left(\sqrt{-\mathcal{K}}\chi\right). \quad (4.5)$$

On using the relation $\sqrt{-\mathcal{K}} = i\sqrt{\mathcal{K}}$ for $\mathcal{K} > 0$, Eq. (4.5) gives $f_{\mathcal{K}}(\chi) = r = (1/\sqrt{\mathcal{K}}) \sin(\sqrt{\mathcal{K}}\chi)$. Taking the limit $\mathcal{K} \rightarrow -0$ in Eq. (4.5), it follows that $f_{\mathcal{K}}(\chi) = \chi$. In summary, the line element on the FLRW background can be expressed as (4.4) in a unified way by using the function (4.5).

A light propagating in the χ direction obeys the geodesic equation

$$ds^2 = -c^2 dt^2 + a^2(t) d\chi^2 = 0. \quad (4.6)$$

Suppose that the light emitted at point χ and time t (redshift z , scale factor a) reaches the observer at point $\chi = 0$ and time t_0 (redshift 0, scale factor a_0). In this case there is the relation $d\chi = -c dt/a(t)$, which is integrated to give $\chi = -\int_{t_0}^t c/a(\tilde{t}) d\tilde{t}$. From Eq. (2.1) we also have the correspondence between t and z , as

$$\frac{dt}{dz} = -\frac{1}{(1+z)H}, \quad (4.7)$$

where $H = \dot{a}/a$ is the Hubble expansion rate. Then, the comoving distance is

$$\chi = \frac{c}{a_0} \int_0^z \frac{d\tilde{z}}{H(\tilde{z})}. \quad (4.8)$$

For the metric (4.4), the change of distance x along the surface associated with the infinitesimal change of angle θ is given by $dx = a(t) f_{\mathcal{K}}(\chi) d\theta$. We define the angular diameter distance, as

$$d_A(t) = \frac{dx}{d\theta} = a(t) f_{\mathcal{K}}(\chi), \quad (4.9)$$

which is often exploited in the distance measurement of CMB observations.

4.2. Friedmann equations

Let us derive the background equations of motion on the FLRW spacetime described by the line element (4.1) with (4.2). On this background, the metric tensor has only

diagonal components, as

$$g_{00} = -1, \quad g_{11} = \frac{a^2(t)}{1 - \mathcal{K}r^2}, \quad g_{22} = a^2(t)r^2, \quad g_{33} = a^2(t)r^2 \sin^2 \theta. \quad (4.10)$$

From Eq. (3.24), the non-vanishing components of Christoffel symbols are

$$\begin{aligned} \Gamma_{ij}^0 &= \frac{1}{c} a^2 H \gamma_{ij}, \quad \Gamma_{0j}^i = \Gamma_{j0}^i = \frac{1}{c} H \delta_j^i, \quad \Gamma_{11}^1 = \frac{\mathcal{K}r}{1 - \mathcal{K}r^2}, \\ \Gamma_{22}^1 &= -r(1 - \mathcal{K}r^2), \quad \Gamma_{33}^1 = -r(1 - \mathcal{K}r^2) \sin^2 \theta, \quad \Gamma_{33}^2 = -\sin \theta \cos \theta, \\ \Gamma_{12}^2 &= \Gamma_{21}^2 = \Gamma_{13}^3 = \Gamma_{31}^3 = \frac{1}{r}, \quad \Gamma_{23}^3 = \Gamma_{32}^3 = \cot \theta. \end{aligned} \quad (4.11)$$

From Eq. (3.52), we obtain non-vanishing components of the Ricci tensor, as

$$R_{00} = -\frac{3}{c^2}(H^2 + \dot{H}), \quad R_{ij} = \frac{a^2}{c^2} \left(3H^2 + \dot{H} + \frac{2\mathcal{K}c^2}{a^2} \right) \gamma_{ij}. \quad (4.12)$$

Then, the Ricci scalar is given by

$$R = \frac{6}{c^2} \left(2H^2 + \dot{H} + \frac{\mathcal{K}c^2}{a^2} \right). \quad (4.13)$$

Finally we obtain non-vanishing components of the Einstein tensor, as

$$G_0^0 = -\frac{3}{c^2} \left(H^2 + \frac{\mathcal{K}c^2}{a^2} \right), \quad G_j^i = -\frac{1}{c^2} \left(3H^2 + 2\dot{H} + \frac{\mathcal{K}c^2}{a^2} \right) \delta_j^i. \quad (4.14)$$

For the matter sector, we take into account a perfect fluid discussed in Sec. 3.3. For the compatibility with the FLRW background, the fluid energy-momentum tensor T_λ^μ should contain only the energy density ρc^2 and the isotropic pressure P , so it is restricted to be of the perfect-fluid form (3.75) with diagonal components alone. Let us consider the Einstein equation (3.85) without the cosmological constant term. From the (00) and (11) components we obtain

$$H^2 = \frac{8\pi G}{3} \rho - \frac{\mathcal{K}c^2}{a^2}, \quad (4.15)$$

$$3H^2 + 2\dot{H} = -8\pi G \frac{P}{c^2} - \frac{\mathcal{K}c^2}{a^2}, \quad (4.16)$$

respectively. The (22) and (33) components of Eq. (3.85) also give rise to Eq. (4.16). Hence we have two independent equations of motion (4.15) and (4.16), which are called Friedmann equations. Eliminating the term $\mathcal{K}c^2/a^2$ from Eqs. (4.15) and (4.16), it follows that

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3} \left(\rho + \frac{3P}{c^2} \right) = -\frac{4\pi G \rho}{3} (1 + 3w), \quad (4.17)$$

where

$$w = \frac{P}{\rho c^2} \quad (4.18)$$

is the equation of state of the perfect fluid. The Universe exhibits the decelerated expansion for $w > -1/3$, while the cosmic acceleration occurs for $w < -1/3$. Eliminating the term H^2 from Eqs. (4.15) and (4.16), we find

$$\dot{H} = -4\pi G\rho(1+w) + \frac{\mathcal{K}c^2}{a^2}. \quad (4.19)$$

In the flat Universe ($\mathcal{K} = 0$) with $\rho > 0$, the Hubble parameter decreases for $w > -1$. If $w = -1$, then H is constant.

Taking the time derivative of Eq. (4.15) and using Eq. (4.16), we obtain

$$\dot{\rho} + 3H\left(\rho + \frac{P}{c^2}\right) = 0, \quad (4.20)$$

which is called the continuity equation. This equation corresponds to the conservation law (3.78) of energy-momentum tensor, i.e.,

$$\nabla_\mu T_0^\mu = \frac{1}{c}\dot{T}_0^0 + \Gamma_{0i}^iT_0^0 - \Gamma_{0i}^iT_i^i = 0. \quad (4.21)$$

After substituting $T_0^0 = -\rho c^2$, $T_j^i = P\delta_j^i$, and $\Gamma_{0j}^i = (H/c)\delta_j^i$ into Eq. (4.21), the continuity equation (4.20) also follows.

In terms of the energy density $\varepsilon = \rho c^2$, we can write the continuity equation (4.20) as the form with an infinitesimal change:

$$d(\varepsilon V) = -PdV, \quad (4.22)$$

where $V = a^3$. Let us consider a matter fluid with an entropy S and an internal energy U in a state of thermal equilibrium with a temperature T . If matter species do not change though chemical reactions (which corresponds to vanishing chemical potentials), then the first law of thermodynamics

$$dU = TdS - PdV \quad (4.23)$$

holds. Now, we can interpret the internal energy as $U = \varepsilon V$, so the entropy conservation ($dS = 0$) follows from Eq. (4.22). We will derive a concrete form of the entropy in Sec. 4.3.

Defining density parameters

$$\Omega_M \equiv \frac{8\pi G\rho}{3H^2}, \quad \Omega_{\mathcal{K}} \equiv -\frac{\mathcal{K}c^2}{(aH)^2}, \quad (4.24)$$

Eq. (4.15) can be expressed in the form

$$\Omega_M + \Omega_K = 1. \quad (4.25)$$

As we will see in Sec. 4.4, the present value of Ω_K is close to 0. The matter density corresponding to the Hubble constant H_0 is given by

$$\rho_0 = \frac{3H_0^2}{8\pi G}, \quad (4.26)$$

which is dubbed the critical density. On using Eq. (2.9) and the value of Newton constant $G = 6.6738 \times 10^{-11} \text{ kg}^{-1} \text{ m}^3 \text{ s}^{-2}$, it follows that

$$\rho_0 = 1.88 h^2 \times 10^{-29} \text{ g cm}^{-3}. \quad (4.27)$$

Then today's average density is about $\rho_0 \approx 10^{-29} \text{ g cm}^{-3}$, which corresponds to the energy density $\varepsilon_0 = \rho_0 c^2 \approx 10^{-15} \text{ J cm}^{-3}$. As we showed in Eq. (2.17), the total energy density of photons in the blackbody radiation is $\varepsilon_\gamma^{(0)} = \pi^2 k_B^4 T_0^4 / [15(\hbar c)^3]$, where $T_0 \simeq 2.725 \text{ K}$. Then, the ratio between $\varepsilon_\gamma^{(0)}$ and ε_0 reads

$$\Omega_\gamma^{(0)} \equiv \frac{\varepsilon_\gamma^{(0)}}{\varepsilon_0} = 2.47 \times 10^{-5} h^{-2}. \quad (4.28)$$

This means that today's energy density of photons is very small compared to the total energy density of the Universe.

We also define the density parameters of matter species (density $\rho_j^{(0)}$ and energy density $\varepsilon_j^{(0)}$) in the present Universe, as

$$\Omega_j^{(0)} \equiv \frac{8\pi G \rho_j^{(0)}}{3H_0^2} = \frac{\rho_j^{(0)}}{\rho_0} = \frac{\varepsilon_j^{(0)}}{\varepsilon_0}. \quad (4.29)$$

In Sec. 4.3, we will enter details for the property of each matter.

4.3. Matter species in the Universe

Matter species present in the today's Universe can be categorized into three classes: (i) relativistic matter, (ii) non-relativistic matter, and (iii) dark energy. In the case (i), the thermal kinetic energy $k_B T$ associated with temperature T is much larger than the rest energy mc^2 of a particle with rest mass m . The main contributions to relativistic matter are photons and neutrinos, whose energy densities are less than 0.01% of the total energy density of the today's Universe. In the case (ii), the particle has a velocity v much smaller than the speed of light c , with the mass satisfying $mc^2 \gg k_B T$. Non-relativistic matter is made of dark matter and baryons, whose energy densities constitute about 30% of the today's total energy density.

Finally, dark energy is an unknown component responsible for the cosmic acceleration. Observationally, it is known that about 70% of today's energy density of the Universe corresponds to dark energy. Dark energy is now the dominant component,

but as we go back to the past, there were epochs in which non-relativistic matter and radiation dominate over other matter components (which are called “matter-dominated” and “radiation-dominated” epochs, respectively). The early Universe was in an equilibrium state filled with relativistic particles.

In statistical thermodynamics, the ensemble of particles with mass m and chemical potential μ in a state of thermal equilibrium with temperature T obeys the distribution function

$$f(\mathbf{p}) = \frac{1}{\exp[(E(\mathbf{p}) - \mu)/(k_B T)] \pm 1}, \quad (4.30)$$

where the particle energy E is related to its momentum $\mathbf{p}$, as $E^2 = \mathbf{p}^2 c^2 + m^2 c^4$. The plus and minus signs of Eq. (4.30) correspond to fermions and bosons, respectively. Generally the distribution function f depends on the particle position $\mathbf{x}$, but since we are now considering the homogenous and isotropic Universe, f is a function of the amplitude p of momentum $\mathbf{p}$ alone. The phase space number in the three-dimensional momentum space $d^3 p$ is given by $d^3 p/(2\pi\hbar)^3$, so the number density n and the energy density ε of a particle with an internal degree of freedom g_* are given, respectively, by

$$n = g_* \int \frac{d^3 p}{(2\pi\hbar)^3} f(p) \quad (4.31)$$

$$= \frac{g_*}{2\pi^2(\hbar c)^3} \int_{mc^2}^{\infty} dE \frac{E \sqrt{E^2 - m^2 c^4}}{\exp[(E - \mu)/(k_B T)] \pm 1}, \quad (4.32)$$

$$\varepsilon = g_* \int \frac{d^3 p}{(2\pi\hbar)^3} E(p) f(p) \quad (4.33)$$

$$= \frac{g_*}{2\pi^2(\hbar c)^3} \int_{mc^2}^{\infty} dE \frac{E^2 \sqrt{E^2 - m^2 c^4}}{\exp[(E - \mu)/(k_B T)] \pm 1}. \quad (4.34)$$

The pressure for each particle with the velocity v is $\tilde{P} = pv/3 = c^2 p^2/(3E)$, where we used the relation $p/E = v/c^2$ in the second equality. Hence the total pressure reads

$$P = g_* \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{c^2 p^2}{3E} f(p) \quad (4.35)$$

$$= \frac{g_*}{6\pi^2(\hbar c)^3} \int_{mc^2}^{\infty} dE \frac{(E^2 - m^2 c^4)^{3/2}}{\exp[(E - \mu)/(k_B T)] \pm 1}. \quad (4.36)$$

Let us first compute n , ε , P for relativistic particles satisfying the condition $k_B T \gg mc^2$. For CMB photons, there exists an observational bound on the chemical potential: $\mu/(k_B T) < 9 \times 10^{-5}$ [1], so we will set $\mu/(k_B T) \rightarrow 0$ in the following discussion. Taking the $m \rightarrow 0$ limit in Eq. (4.32) and setting $x = E/(k_B T)$, the

number density reduces to

$$n = \frac{g_*(k_B T)^3}{2\pi^2(\hbar c)^3} \int_0^\infty dx \frac{x^2}{e^x \pm 1} = \frac{\zeta(3)g_*(k_B T)^3}{\pi^2(\hbar c)^3} \times \begin{cases} 1 & (\text{boson}), \\ 3/4 & (\text{fermion}), \end{cases} \quad (4.37)$$

where $\zeta(3) = 1.202 \dots$ is the Riemann zeta function. Similarly, the computation of integrals (4.34) and (4.36) gives

$$\varepsilon = \frac{\pi^2 g_*(k_B T)^4}{30(\hbar c)^3} \times \begin{cases} 1 & (\text{boson}), \\ 7/8 & (\text{fermion}), \end{cases} \quad (4.38)$$

$$P = \frac{\varepsilon}{3}. \quad (4.39)$$

Then, the equation of state $w = P/\varepsilon$ of radiation is given by

$$w = \frac{1}{3}. \quad (4.40)$$

The photon is a bosonic particle with two spin states ($g_* = 2$), so the energy density reduces to the result (2.17).

Let us next proceed to the calculations of n , ε , P for non-relativistic particles ($mc^2 \gg k_B T$). In this case we have that $\exp[(E - \mu)/(k_B T)] \gg 1$, so there is no difference between bosons and fermions. On using the approximation $E \simeq mc^2 + p^2/(2m)$, we obtain the number density

$$\begin{aligned} n &\simeq \frac{g_*}{2\pi^2 \hbar^3} e^{-(mc^2 - \mu)/(k_B T)} \int_0^\infty dp p^2 e^{-p^2/(2mk_B T)} \\ &= g_* \left(\frac{mk_B T}{2\pi \hbar^2} \right)^{3/2} e^{-(mc^2 - \mu)/(k_B T)}. \end{aligned} \quad (4.41)$$

Similarly, we can express ε and P in terms of n as

$$\varepsilon \simeq nmc^2, \quad (4.42)$$

$$P \simeq nk_B T \simeq \frac{k_B T}{mc^2} \varepsilon. \quad (4.43)$$

Then the equation of state of non-relativistic matter is

$$w = \frac{k_B T}{mc^2}, \quad (4.44)$$

and hence $w \simeq 0$.

Before entering the detail of each particle, we derive an explicit form of the entropy mentioned in Sec. 4.2. As long as the chemical potential μ is much smaller than E , taking the partial derivative of the distribution function (4.30) with respect to T leads to

$$\frac{\partial f}{\partial T} = -\frac{E}{T} \frac{\partial f}{\partial E} = -\frac{1}{T} \frac{E^2}{pc^2} \frac{\partial f}{\partial p}. \quad (4.45)$$

Using this relation, the partial derivative of the pressure (4.35) in terms of T reads

$$\frac{\partial P}{\partial T} = -\frac{g_*}{3T} \int \frac{d^3p}{(2\pi\hbar)^3} pE \frac{\partial f}{\partial p} = \frac{\varepsilon + P}{T}. \quad (4.46)$$

In the last equality of Eq. (4.46), we have carried out the partial integral with respect to p and employed the definition of ε given in Eq. (4.33). Since the first law of thermodynamics corresponds to $TdS = d(\varepsilon V) + PdV$, the variation of S gives

$$dS = \frac{1}{T} [d((\varepsilon + P)V) - VdP] = d \left[\frac{(\varepsilon + P)V}{T} \right], \quad (4.47)$$

where we used Eq. (4.46). Then, the entropy can be explicitly written as

$$S = \frac{(\varepsilon + P)V}{T}. \quad (4.48)$$

Since $dS = 0$ under the relation (4.22), the entropy of a perfect fluid is conserved on the FLRW background.

In the following, we enter the details for relativistic particles, non-relativistic particles, and dark energy, respectively.

4.3.1. *Relativistic particles*

Among relativistic particles, we already derived the density parameter $\Omega_\gamma^{(0)}$ of photons in Eq. (4.28).

Besides photons, neutrinos can also behave as relativistic particles today. Neutrinos are fermions that interact very weakly with standard model particles. They arise in states of three flavors: electron neutrinos (ν_e), muon neutrinos (ν_μ), and tau neutrinos (ν_τ). Each flavor also has antiparticles, i.e., $\bar{\nu}_e$, $\bar{\nu}_\mu$, and $\bar{\nu}_\tau$. Experimentally, it is known that neutrinos can oscillate from one flavor to another, which requires non-vanishing mass terms. Neutrino oscillations arise from a mixing between flavor and mass eigenstates (labelled by 1,2,3) of them.

From neutrino-oscillation experiments the neutrino mass itself cannot be determined, but the mass difference between two different mass eigenstates are constrained. The atmospheric neutrino experiments such as Super-Kamiokande and solar neutrino experiments combined with KamLAND put constraints on the mass difference to be $\Delta m_{12}^2 = 7.53_{-0.18}^{+0.18} \times 10^{-5} \text{ eV}^2$ and $\Delta m_{31}^2 \simeq \Delta m_{32}^2 = 2.44_{-0.06}^{+0.06} \times 10^{-3} \text{ eV}^2$ [2]. The latter bound shows that there exists at least one neutrino mass eigenstate with a mass of the order of 0.05 eV.

In the following, we estimate the average temperature T_ν of neutrinos in the present Universe. Around the onset of nucleosynthesis in the early Universe, the positron (e^+) and the electron (e^-) annihilated to two photons (γ) according to the reaction: $e^+ + e^- \rightarrow \gamma + \gamma$. This annihilation of e^+ and e^- occurred when the electron

became non-relativistic, i.e., when the rest energy of electrons ($m_e c^2 = 0.511$ MeV) became equivalent to the thermal energy $k_B T_{\text{NR}}$, i.e.,

$$T_{\text{NR}} = 0.511 \text{ MeV}/k_B = 5.9 \times 10^9 \text{ K}. \quad (4.49)$$

In the early Universe, neutrinos were in a state of thermal equilibrium with other particles (e^+, e^-), but they started to decouple from the equilibrium state when the rate of neutrino interactions decreased down to the Hubble expansion rate H . Generally, the rate of particle interactions can be written as

$$\Gamma = n\sigma v, \quad (4.50)$$

where n is the number density of particles, σ is their cross-section, and v is the average velocity of particles. For the reactions $\nu_e + e^+ \leftrightarrow \bar{\nu}_e + e^+$, $\bar{\nu}_e + e^- \leftrightarrow \nu_e + e^-$, the cross-section can be estimated as $\sigma \simeq G_F^2 T^2$ from the Fermi's theory of weak interactions [3], where $G_F = 1.166 \times 10^{-5} \text{ GeV}^{-2}$ is the Fermi coupling constant. To derive the ratio Γ/H , we use the natural unit $\hbar = c = k_B = 1$. As we will show in the following, the decoupling of neutrinos occurred at the temperature around 10^{10} K. Just before the decoupling, the internal degrees of freedom of neutrinos, anti-neutrinos, electrons, positrons (all relativistic) are given, respectively, by 3, 3, 2, 2, i.e., $g_* = 10$ in total. Substituting $g_* = 10$ into the fermionic case of Eq. (4.37), the total number density of these particles is $n = 15\zeta(3)T^3/(2\pi^2)$. Since $v \simeq 1$ for relativistic particles, the rate of neutrino interactions is given by

$$\Gamma \simeq \frac{15\zeta(3)G_F^2 T^5}{2\pi^2}. \quad (4.51)$$

For the temperature around $1 \text{ MeV} \lesssim T \lesssim 100 \text{ MeV}$, the relativistic particles contributing to the energy density (4.38) are photons (bosons) besides neutrinos, anti-neutrinos, electrons, positrons (fermions), so the total radiation energy density is given by $\varepsilon_r = \pi^2 g_* T^4/30$, where $g_* = 10.75$. Ignoring the spatial curvature $\mathcal{K}$ in Eq. (4.15) and setting $\rho = \pi^2 g_* T^4/30$, the Hubble parameter can be estimated as

$$H = \sqrt{\frac{4\pi^3 g_*}{45}} \frac{T^2}{m_{\text{pl}}}, \quad (4.52)$$

where m_{pl} is the Planck mass defined by Eq. (1.8). In the natural unit the gravitational constant G is related to the Planck mass, as $G = 1/m_{\text{pl}}^2$. Taking the ratio between (4.51) and (4.52), it follows that

$$\frac{\Gamma}{H} \simeq \left(\frac{k_B T}{1.5 \text{ MeV}} \right)^3, \quad (4.53)$$

where we restored the Boltzmann constant k_B . Hence neutrinos were decoupled from the thermal equilibrium at the temperature $T_{\text{de}} \simeq 1.5 \text{ MeV}/k_B = 1.7 \times 10^{10} \text{ K}$. For the temperature smaller than T_{de} , the entropy produced by the annihilation of e^+

and e^- was transformed only to photons. This implies that, after the positron–electron annihilation, the neutrino temperature T_ν should be smaller than the photon temperature T_γ .

In what follows, we obtain the relation between T_ν and T_γ from the entropy conservation before and after the positron–electron annihilation. From Eq. (4.48) we define the entropy per volume, as

$$s = \frac{\varepsilon + P}{T}. \quad (4.54)$$

Using Eqs. (4.38) and (4.39) for relativistic particles, it follows that

$$s = \frac{2\pi^2 g_* k_B^4 T^3}{45(\hbar c)^3} \times \begin{cases} 1 & (\text{boson}) \\ 7/8 & (\text{fermion}), \end{cases} \quad (4.55)$$

so the entropy has the dependence $S \propto s a^3 \propto g_* T^3 a^3$.

Before positrons and electrons annihilated, photons ($g_* = 2$), positrons ($g_* = 2$), electrons ($g_* = 2$), and three flavors of neutrinos and anti-neutrinos ($g_* = 1$ for each) behaved as relativistic particles. Before the annihilation, we write the temperature and the scale factor of photons and neutrinos as T_1 and a_1 respectively. Then, the entropy of all relativistic particles is given by

$$S(a_1) = \frac{2\pi^2 k_B^4 T_1^3}{45(\hbar c)^3} a_1^3 \left[2 + \frac{7}{8}(2 + 2 + 3 \times 2) \right] = \frac{43}{90} \frac{\pi^2 k_B^4 T_1^3 a_1^3}{(\hbar c)^3}. \quad (4.56)$$

After the positron–electron annihilation (scale factor a_2), the entropy reads

$$S(a_2) = \frac{2\pi^2 k_B^4}{45(\hbar c)^3} a_2^3 \left(2T_\gamma^3 + \frac{7}{8} \cdot 6T_\nu^3 \right), \quad (4.57)$$

where T_ν and T_γ are the temperatures of neutrinos and photons, respectively. Note that there is the relation $a_1 T_1 = a_2 T_\nu$. Since $S(a_1) = S(a_2)$ from the entropy conservation, we obtain

$$\frac{T_\nu}{T_\gamma} = \left(\frac{4}{11} \right)^{1/3}. \quad (4.58)$$

Recall that, even after the decoupling of photons, we can define the photon temperature as Eq. (2.13), so the relation (4.58) can be used even today. For today's photon temperature $T_\gamma^{(0)} = 2.725$ K, the neutrino temperature is given by $T_\nu^{(0)} = 1.945$ K. The mass of neutrinos that have been relativistic up to the present Universe satisfies

$$m_\nu < k_B T_\nu^{(0)} / c^2 = 1.7 \times 10^{-4} \text{ eV} / c^2. \quad (4.59)$$

Let us consider N_{eff} relativistic degrees of freedom of fermions whose temperature obeys the same relation as T_ν in Eq. (4.58) after the positron–electron

annihilation. From Eq. (4.38), the total energy density of relativistic fermions with temperature T_ν yields

$$\varepsilon_\nu = N_{\text{eff}} \frac{7\pi^2 (k_B T_\nu)^4}{120(\hbar c)^3}, \quad (4.60)$$

where the contribution of antiparticles has been taken into account. For the derivation of Eq. (4.60), we ignored the chemical potential μ_ν relative to T_ν . On using Eqs. (2.17), (4.58) and (4.60), the ratio between the energy densities of neutrinos and photons is given by

$$\frac{\varepsilon_\nu}{\varepsilon_\gamma} = \frac{7}{8} \left(\frac{4}{11} \right)^{4/3} N_{\text{eff}}. \quad (4.61)$$

Then, the total density parameter of radiation in the present Universe reads

$$\Omega_r^{(0)} = \Omega_\gamma^{(0)} (1 + 0.2271 N_{\text{eff}}), \quad (4.62)$$

where $\Omega_\gamma^{(0)}$ is given by Eq. (4.28). If the mass of neutrinos is negligible, then $N_{\text{eff}} = 3$. Taking into account the effect that the distribution function of neutrinos is modified at the annihilation epoch of positrons and electrons, the relativistic degree of freedom is modified to $N_{\text{eff}} = 3.046$ [4]. Substituting $N_{\text{eff}} = 3.046$ and $h = 0.68$ into Eq. (4.62), we have $\Omega_r^{(0)} = 9.04 \times 10^{-5}$, so today's radiation energy density constitutes only 0.01% of the total energy density of the Universe.

4.3.2. *Non-relativistic particles*

We consider particles that became non-relativistic today. The first example is baryons. We use the word “baryons” not only for protons and neutrons but also for leptons like electrons (reflecting the fact that masses of leptons are negligibly small relative to those of protons and neutrons). Today's density parameter $\Omega_b^{(0)}$ of baryons can be constrained from the Big Bang nucleosynthesis and the CMB.

The amount of light elements produced during the Big Bang nucleosynthesis is affected by that of baryons. The amount of baryons can be estimated by measuring the mass ratio between light elements of primordial origins. For example, the observations of absorption lines of quasars showed that the mass ratio between deuterium and hydrogen is constrained to be $D/H = (2.78 \pm 0.29) \times 10^{-5}$ [5]. From this, the present density parameter of baryons $\Omega_b^{(0)}$ is constrained to be around 0.04–0.05.

The observations of CMB temperature anisotropies also placed tight constraints on $\Omega_b^{(0)}$. In the radiation-dominated epoch, baryons were tightly coupled to photons. For larger $\Omega_b^{(0)}$, the sound speed c_s associated with the coupled baryon–photon fluid gets smaller. The angular frequency of CMB acoustic oscillations in temperature anisotropies is approximately given by $\omega_k \approx c_s k$. As we will see in Sec. 7.11, the amplitude of CMB acoustic peaks tends to be larger for smaller c_s . From the observations of CMB temperature anisotropies by the Planck collaboration, the baryon

density parameter is constrained to be [6]

$$\Omega_b^{(0)} h^2 = 0.02205 \pm 0.00028 \quad (68\% \text{ CL}), \quad (4.63)$$

where 68% CL means a 68% statistical confidence level. For $h = 0.68$, the central value of Eq. (4.63) corresponds to $\Omega_b^{(0)} = 0.0477$. This is consistent with the bound from the Big Bang nucleosynthesis.

Let us estimate the ratio n_b/n_γ between the baryon number density n_b and the photon number density n_γ . After the baryons are decoupled from the thermal equilibrium in the early Universe, they are described by non-relativistic particles whose number densities decrease as $n_b \propto a^{-3} \propto T^3$. For today's baryon number density $n_b^{(0)}$ and the proton mass m_p , we have $\Omega_b^{(0)} = \rho_b^{(0)}/\rho_0 = m_p n_b^{(0)}/\rho_0$. Then, the baryon number density at temperature T yields

$$n_b = n_b^{(0)} \left(\frac{T}{T_0} \right)^3 = \Omega_b^{(0)} \frac{\rho_0}{m_p} \left(\frac{T}{T_0} \right)^3, \quad (4.64)$$

where ρ_0 is given by Eq. (4.27). From Eq. (4.37), the photon number density reads $n_\gamma = 2\zeta(3)(k_B T)^3/(\pi^2 \hbar^3 c^3)$, so the baryon-to-photon ratio n_b/n_γ is given by

$$\eta_b \equiv \frac{n_b}{n_\gamma} = \frac{\pi^2}{2\zeta(3)} \frac{\rho_0}{m_p} \frac{(\hbar c)^3}{(k_B T_0)^3} \Omega_b^{(0)}, \quad (4.65)$$

which is constant. On using the values $m_p = 1.673 \times 10^{-27}$ kg, $T_0 = 2.725$ K, and Eq. (4.27), it follows that

$$\eta_b = 2.7 \times 10^{-8} \Omega_b^{(0)} h^2. \quad (4.66)$$

For the central value of Eq. (4.63), we have $\eta_b \simeq 6 \times 10^{-10}$. Hence the number density of baryons is much smaller than that of photons.

The existence of baryons alone is not sufficient to explain observed large-scale structures in the Universe. We need another source of non-relativistic matter called dark matter for the consistency with observations. Dark matter clusters due to gravitational interactions. However, they do not interact through electromagnetic interactions, so it is difficult to directly observe dark matter through light. In 1933, Zwicky indirectly found the existence of dark matter by observing the movement of galaxies in the Coma cluster. Dark matter exerts gravitational forces on galaxies in such a way that the rotational velocities of galaxies do not decrease even in the region far outside a central bright region in clusters.

Usually we classify dark matter into two classes: (i) hot dark matter (HDM) where dark matter is relativistic at the decoupling epoch of CMB photons (which occurred at the redshift $z \simeq 1090$ as we will see in Sec. 7.1), and (ii) cold dark matter (CDM) where dark matter is non-relativistic at the decoupling epoch. One of the representative examples of HDM is the massive neutrino. Since the temperature of neutrinos at the redshift $z = 1090$ can be estimated as $T_{\nu*} = 1.945 \times 1091 \text{ K} = 2.1 \times 10^3 \text{ K}$, the mass of neutrinos relativistic at the decoupling satisfies the condition

$m_\nu < k_B T_{\nu*}/c^2 = 0.18 \text{ eV}/c^2$. The velocity dispersion of neutrinos is large due to its free streaming, in which case it is difficult to cause gravitational clusterings. The suppression of gravitational growth induced by the free movement of particles is called the free-streaming damping. The gravitational clustering driven by the HDM alone cannot explain observed large-scale structures of the Universe.

For the CDM, the free-streaming damping is absent, so it can be the source for the structure formation. Baryons were tightly coupled to photons by the decoupling epoch, so baryon perturbations started to grow after the decoupling. On the other hand, the interactions of CDM with other particles are very small except for the gravitational force, so the growth of CDM perturbations began to occur even before the decoupling epoch. The gravitational clustering induced by CDM has a bottom-up property that small-scale structures were first formed and then they gathered to form larger structures. The structure formation driven by CDM perturbations is not only consistent with observations of large-scale structures but also with other observations such as CMB. From the observations of CMB temperature anisotropies by the Planck team, today's density parameter of CDM is constrained to be [6]

$$\Omega_c^{(0)} h^2 = 0.1199 \pm 0.0027 \quad (68\% \text{ CL}), \quad (4.67)$$

which is about five times as large as the baryon density parameter given by Eq. (4.63). For $h = 0.68$, the central value of Eq. (4.67) is $\Omega_c^{(0)} = 0.2593$.

There is a structure-formation scenario of mixed dark matter in which CDM and HDM coexist, but the amount of HDM is constrained to be less than a few percent for the consistency with observations of large-scale structures. For instance, let us consider a massive neutrino with mass m_ν . The massive neutrino that is non-relativistic today satisfies the opposite inequality to Eq. (4.59), i.e., $m_\nu > 1.7 \times 10^{-4} \text{ eV}/c^2$. For neutrinos that were relativistic at its decoupling epoch ($T_{\text{de}} \simeq 1.5 \text{ MeV}/k_B$), the mass is in the range $m_\nu < 1.5 \text{ MeV}/c^2$. Even after the neutrino decoupling, its number density is given by that of fermions in Eq. (4.37) with the temperature $T_\nu = T_{\text{de}} (a_{\text{de}}/a)$. Then, the total number density of neutrinos and anti-neutrinos is

$$n_\nu(T_\nu) = \frac{3\zeta(3)(k_B T_\nu)^3}{2\pi^2(\hbar c)^3}. \quad (4.68)$$

After the neutrino became non-relativistic, its number density decreased in the same way as Eq. (4.68), i.e., in proportion to a^{-3} . Then, today's number density is given by

$$n_\nu^{(0)} = \frac{3\zeta(3)(k_B T_\nu^{(0)})^3}{2\pi^2(\hbar c)^3} = 112 \text{ cm}^{-3}, \quad (4.69)$$

where, in the second equality, we used $T_\nu^{(0)} = 1.945 \text{ K}$. Since today's density of non-relativistic neutrinos is $\rho_\nu^{(0)} = \sum n_\nu^{(0)} m_\nu$, the corresponding density

parameter is

$$\Omega_{\nu,\text{NR}}^{(0)} = \frac{\rho_{\nu}^{(0)}}{\rho_0} = \frac{\sum m_{\nu}}{94 \text{ eV}/c^2}. \quad (4.70)$$

From the Planck CMB data, there is the constraint $\sum m_{\nu} < 0.23 \text{ eV}/c^2$ (95% CL) [6], so the density parameter of non-relativistic neutrinos is constrained to be $\Omega_{\nu,\text{NR}}^{(0)} < 2.4 \times 10^{-3}$.

There are several candidates for CDM, which are mostly particles appearing in theories beyond the Standard Model (SM) of particle physics. In supersymmetric theories (including superstring and supergravity theories), for example, each particle arising in SM has a heavier partner of different spin but a similar interaction. The lightest of these new particles is usually stable in the presence of symmetry called the R-parity. This class of CDM candidates is generally called the weakly interacting massive particles (WIMPs) [7]. One example of WIMPs is a neutralino with mass of the order of $10 \sim 10^4 \text{ GeV}$, which is composed of super-partners of Z-boson, photon, and Higgs particle.

Another candidate for CDM is an axion, which was originally introduced to solve a strong charge-parity (CP) problem in quantum chromodynamics (QCD). In the original model of Peccei and Quinn [8], the axion does not work as CDM. However, in extended models [9, 10], the axion can be the source for CDM for the mass range $10^{-5} \text{ eV}/c^2 \lesssim m_a \lesssim 10^{-2} \text{ eV}/c^2$. Dark matter having properties between CDM and HDM is called warm dark matter (WDM). The candidates for WDM are gravitinos (supersymmetric partner of gravitons) and sterile neutrinos (which do not have weak interactions).

There have been numerous efforts for finding the signature of dark matter in experiments, but we have not succeeded its detection yet. It remains to be seen whether ongoing and future experiments can reveal the origin of dark matter. Readers may have a look at Vol. 4 Dark Matter of the encyclopedia [11] for theoretical and experimental aspects of dark matter.

4.3.3. Dark energy

Dark energy, which is responsible for the late-time cosmic acceleration, constitutes about 70% of the present energy density of the Universe. Dark energy has a negative pressure with the equation of state w_{DE} smaller than $-1/3$. The simplest candidate for dark energy is the cosmological constant Λ ; see Eq. (3.86). If we move the term $\Lambda g_{\mu\nu}$ to the right hand side of Eq. (3.86), it can be interpreted as a term with the density $\rho = \Lambda c^2/(8\pi G)$ and the pressure $P = -\Lambda c^4/(8\pi G)$. Then, the equation of state of the cosmological constant corresponds to $w_{\text{DE}} = -1$. In this case, today's density parameter of dark energy is observationally constrained to be [6]

$$\Omega_{\text{DE}}^{(0)} = 0.685_{-0.016}^{+0.018} \quad (68\% \text{ CL}). \quad (4.71)$$

If the origin of dark energy is not the cosmological constant, the equation of state is generally different from 1. As we will see later in detail, models of dark energy can be broadly classified into two classes: (i) specific matter sources with negative pressures, and (ii) modifying gravity from GR. Since the evolution of w_{DE} is different depending on models of dark energy, it is possible to distinguish between them from observations. The cosmological constant has been consistent with numerous observational data. Dynamical dark energy models in which w_{DE} does not significantly deviate from -1 have not been excluded from the data. The model in which the cosmological constant and the cold dark matter are two dark components of the Universe is dubbed the Λ CDM model.

4.4. Cosmic expansion history from the radiation era

Let us consider a fluid with a constant equation of state $w = P/(\rho c^2)$. In this case, Eq. (4.20) can be integrated to give

$$\rho \propto a^{-3(1+w)}. \quad (4.72)$$

Since $w = 1/3$ for relativistic particles in thermal equilibrium, the radiation energy density decreases as $\varepsilon_r = \rho_r c^2 \propto a^{-4}$. As we showed in Eq. (2.17) for photons, ε_r is proportional to T^4 , so the temperature decreases as

$$T \propto a^{-1}. \quad (4.73)$$

For non-relativistic matter we have $w \simeq 0$, so the matter density evolves as $\rho_m \propto a^{-3}$. This corresponds to the conservation of mass: $\rho_m a^3 = \text{constant}$.

In the flat Universe, the Friedmann equation (4.15) reduces to $3H^2 = 8\pi G\rho$. Substituting Eq. (4.72) into the Friedmann equation and integrating it for $w > -1$, we obtain the expanding solution

$$a \propto t^{2/[3(1+w)]}. \quad (4.74)$$

During the radiation-dominated epoch in which relativistic particles are the dominant contribution to the total energy density, the scale factor evolves as $a \propto t^{1/2}$. In the matter-dominated epoch where non-relativistic particles dominate the total energy density, the evolution of scale factor is given by $a \propto t^{2/3}$ (as it matches with the result of Newton gravity in Sec. 2.3). For $-1 < w < -1/3$, the Universe exhibits an acceleration. The cosmological constant corresponds to $w = -1$, in which case ρ is constant from Eq. (4.72). Since $H = \dot{a}/a$ is constant in the Universe dominated by the cosmological constant, we obtain the solution $a \propto e^{Ht}$. As we will see in Sec. 4.6, there was an epoch of cosmic acceleration (inflation) which occurred prior to the radiation-dominated epoch.

For $w < -1$, the solution (4.74) corresponds to a collapsing Universe in which a decreases with time. In this case, the expanding solution is given by

$$a \propto (t_s - t)^{2/[3(1+w)]}, \quad (4.75)$$

where t_s is a constant. The solution (4.75) is valid for $t < t_s$. As t approaches t_s , the scale factor and the Ricci scalar diverge at $t = t_s$. Then, the Universe ends at a big rip singularity [12]. The dark energy equation of state w_{DE} smaller than -1 is allowed from observations, but in the framework of GR it is difficult to realize $w_{\text{DE}} < -1$ without theoretical problems like the appearance of ghosts. In modified gravity theories, however, it is possible to have $w_{\text{DE}} < -1$ without ghosts.

The cosmic expansion history is characterized by the sequence of (a) inflationary era, (b) radiation-dominated epoch, (c) matter-dominated epoch, and (d) dark energy-dominated epoch. Let us consider the cosmological evolution after the onset of radiation domination. Then, we consider three matter species: (i) radiation (density ρ_r), (ii) non-relativistic matter (density ρ_m), and (iii) dark energy (density ρ_{DE}). From the Friedmann equation (4.15) it follows that

$$H^2 = \frac{8\pi G}{3}(\rho_r + \rho_m + \rho_{\text{DE}}) - \frac{\mathcal{K}c^2}{a^2}. \quad (4.76)$$

Now, we rewrite Eq. (4.76) in terms of the redshift $z = a_0/a - 1$. Since there is the relation $dt/dz = -1/[H(1+z)]$ between z and the cosmic time t , we can express Eq. (4.20) in the integrated form

$$\rho(z) = \rho^{(0)} \exp \left[\int_0^z \frac{3\{1 + w(\tilde{z})\}}{1 + \tilde{z}} d\tilde{z} \right], \quad (4.77)$$

where $\rho^{(0)}$ is today's value of ρ (at $z = 0$). Note that Eq. (4.77) is valid for a time-varying equation of state w .

For radiation ($w = 1/3$) and non-relativistic matter ($w = 0$), we can explicitly integrate Eq. (4.77) to give $\rho_r = \rho_r^{(0)}(1+z)^4$ and $\rho_m = \rho_m^{(0)}(1+z)^3$, respectively. For dark energy whether w_{DE} is constant or not is unknown, so we express its density in the form (4.77), i.e., $\rho_{\text{DE}}(z) = \rho_{\text{DE}}^{(0)} \exp \left[\int_0^z 3\{1 + w_{\text{DE}}(\tilde{z})\}/(1 + \tilde{z}) d\tilde{z} \right]$. According to Eq. (4.29), today's density parameters of radiation, non-relativistic matter, and dark energy are defined respectively, as $\Omega_r^{(0)}$, $\Omega_m^{(0)}$, and $\Omega_{\text{DE}}^{(0)}$. The density parameter associated with the spatial curvature $\mathcal{K}$ is given by $\Omega_{\mathcal{K}}^{(0)} = -\mathcal{K}c^2/(a_0^2 H_0^2)$. Then, the Hubble parameter squared (4.76) can be written as

$$H^2(z) = H_0^2 \left[\Omega_r^{(0)}(1+z)^4 + \Omega_m^{(0)}(1+z)^3 + \Omega_{\text{DE}}^{(0)} \exp \left\{ \int_0^z \frac{3\{1 + w_{\text{DE}}(\tilde{z})\}}{1 + \tilde{z}} d\tilde{z} \right\} + \Omega_{\mathcal{K}}^{(0)}(1+z)^2 \right]. \quad (4.78)$$

At $z = 0$, there is the relation $\Omega_r^{(0)} + \Omega_m^{(0)} + \Omega_{\text{DE}}^{(0)} + \Omega_{\mathcal{K}}^{(0)} = 1$. If w_{DE} is constant, the third term in the parenthesis of Eq. (4.78) reduces to $\Omega_{\text{DE}}^{(0)}(1+z)^{3(1+w_{\text{DE}})}$. The present Universe is dominated by dark energy with $\Omega_{\text{DE}}^{(0)}$ given by Eq. (4.71). Since w_{DE} is close to -1 , the contribution $\Omega_{\text{DE}}^{(0)}(1+z)^{3(1+w_{\text{DE}})}$ does not grow much in

the past. For $w_{\text{DE}} = \text{constant}$, the redshift z_c at which the energy densities of dark energy and non-relativistic matter are equivalent to each other is given by

$$z_c = \left(\frac{\Omega_m^{(0)}}{\Omega_{\text{DE}}^{(0)}} \right)^{1/(3w_{\text{DE}})} - 1. \quad (4.79)$$

If $w_{\text{DE}} = -1$, $\Omega_{\text{DE}}^{(0)} = 0.69$, and $\Omega_m^{(0)} = 0.31$, for example, then $z_c = 0.31$. For $z > z_c$, the energy density of non-relativistic matter is larger than that of dark energy.

The present density parameter $\Omega_r^{(0)}$ of radiation is as small as 0.01, but as we go back to the past, the first contribution inside the parenthesis of Eq. (4.78) tends to dominate over other terms. On using the value $N_{\text{eff}} = 3.046$ in Eq. (4.62), the redshift z_{eq} at which the energy density of radiation became equivalent to that of non-relativistic matter is given by

$$z_{\text{eq}} = 2.40 \times 10^4 \Omega_m^{(0)} h^2 - 1, \quad (4.80)$$

where $\Omega_m^{(0)} = \Omega_b^{(0)} + \Omega_c^{(0)}$. If we adopt the central values of (4.63) and (4.67), we have $\Omega_m^{(0)} h^2 = 0.142$ and hence $z_{\text{eq}} = 3400$. At the redshift $z > z_{\text{eq}}$, the Universe was dominated by the radiation.

As we go back to the past, the spatial curvature term $\Omega_{\mathcal{K}}^{(0)}(1+z)^2$ in Eq. (4.78) also gets larger. In the Λ CDM model, the Planck CMB data showed that the spatial curvature is constrained to be

$$\Omega_{\mathcal{K}}^{(0)} = -0.0010_{-0.0065}^{+0.0062} \quad (95\% \text{ CL}), \quad (4.81)$$

which means that the present Universe is close to a flat state. The contributions of non-relativistic matter and radiation to the right hand side of Eq. (4.78) increase faster than that of spatial curvature, so the curvature term does not dominate over the former in the past.

We define the effective equation of state of the Universe, as

$$w_{\text{eff}} \equiv -1 - \frac{2\dot{H}}{3H^2} = -1 + \frac{2(1+z)}{3H} \frac{dH}{dz}. \quad (4.82)$$

In the Universe dominated by a j -component of matter (with an equation of state w_j), we have that $H^2(z) = H_0^2 \Omega_j^{(0)} \exp \left[\int_0^z 3\{1 + w_j(\tilde{z})\}/(1 + \tilde{z}) d\tilde{z} \right]$. During the sequence of radiation, matter, and dark energy dominated epochs, the effective equation of state changes as $1/3 \rightarrow 0 \rightarrow w_{\text{DE}}$. Taking the z derivative of Eq. (4.78), the dark energy equation of state can be expressed as

$$w_{\text{DE}}(z) = \frac{(1+z)(E^2(z))' - 3E^2(z) - \Omega_r^{(0)}(1+z)^4 + \Omega_{\mathcal{K}}^{(0)}(1+z)^2}{3 \left[E^2(z) - \Omega_r^{(0)}(1+z)^4 - \Omega_m^{(0)}(1+z)^3 - \Omega_{\mathcal{K}}^{(0)}(1+z)^2 \right]}, \quad (4.83)$$

where $E(z) \equiv H(z)/H_0$ and a prime represents a derivative with respect to z . As we will see in Sec. 5.3, the quantity $E(z)$ is related to the luminosity distance $d_L(z)$

from an observer to an astronomical object. In SN Ia observations, the property of dark energy can be constrained by measuring $d_L(z)$ at many different redshifts.

4.5. Planck era

If we go back to the asymptotic past even before the radiation era, GR predicts a Big Bang singularity associated with the divergence of curvature. However, GR is a classical theory without taking into account quantum effects of spacetime. Quantum theory of gravity (quantum gravity) was not successfully constructed yet, but there is a possibility that the singularity problem can be resolved after the completion of quantum gravity.

Let us estimate the energy scale (called the Planck scale) above which the spacetime itself should be treated in a quantum mechanical way. In doing so, we consider a flat Universe dominated by matter with the density ρ and the pressure P . We assume that the equation of state $w = P/(\rho c^2)$ is larger than -1 . For constant w , the evolution of the Hubble parameter is given by $H \sim 1/t$ with the density $\rho \sim H^2/G$. The energy inside the Hubble radius $L_H = cH^{-1}$ corresponds to $E = \rho c^2 L_H^3 \sim c^5/(GH)$. The product of E and t is given by $Et \sim (c^5/G)t^2$, so the time t_{pl} at which Et is equivalent to $\hbar$ is given as

$$t_{\text{pl}} = \sqrt{\frac{\hbar G}{c^5}} = 5.3911 \times 10^{-44} \text{ s}, \quad (4.84)$$

which is called the Planck time. The energy associated with t_{pl} is given by $E_{\text{pl}} = \hbar/t_{\text{pl}} = \sqrt{\hbar c^5/G}$. For $t \lesssim t_{\text{pl}}$, quantum effects of spacetime cannot be ignored due to an uncertainty principle. If we interpret the Planck time (4.84) in terms of the length scale $\ell_{\text{pl}} = ct_{\text{pl}}$ and the mass scale $m_{\text{pl}} = E_{\text{pl}}/c^2$, they are given, respectively, by Eqs. (1.6) and (1.8). For the energy scale higher than $E_{\text{pl}} \simeq 10^{19}$ GeV, it is expected that quantum field theory is unified with GR. String theory and loop quantum gravity are the candidates for such a unified theory. Gravity, which is weakest among four known forces in Nature, first separated from other forces around the Planck scale.

4.6. Inflation

In Sec. 4.4, we showed that the Universe was dominated by radiation at redshifts larger than $z_{\text{eq}} \approx 3400$. Prior to the radiation-dominated epoch, it is believed that there were epochs of inflation and reheating. The idea of inflation was originally proposed to address several problems of the Big Bang cosmology — such as flatness and horizon problems (as we will explain in Sec. 4.6.1). Moreover, the observations of CMB temperature anisotropies are consistent with the primordial power spectrum of curvature perturbations generated during inflation. As we will see in Sec. 6.8, the typical energy scale of inflation can be estimated as 10^{14} GeV from the amplitude of

CMB fluctuations. This is lower than the Planck scale, but it is much higher than the electroweak scale ($\sim 10^2$ GeV). The realization of inflation usually requires the presence of a scalar field beyond the standard model of particle physics.

4.6.1. Resolving the flatness and horizon problems

Today's density parameter of spatial curvature is constrained as Eq. (4.81), so today's Universe is nearly flat. During the radiation and matter eras the Universe exhibited decelerated expansions, such that the scale factor evolved as $a \propto t^p$ ($0 < p < 1$). In this case the evolution of the Hubble parameter is given by $H = p/t$, so $|\Omega_K| = |K|/(a^2 H^2)$ grows in proportion to $\propto t^{2(1-p)}$. To realize a small value of $\Omega_K^{(0)}$ consistent with the bound (4.81), we require that $|\Omega_K|$ is very much smaller than 1 in the very early Universe. In the Planck era, for example, $|\Omega_K| \lesssim 10^{-66}$. This fine tuning of the spatial curvature is called the flatness problem. The Universe entered the dark-energy dominated epoch for the redshift $z \lesssim \mathcal{O}(1)$, but the period of this late-time acceleration is too short to solve the flatness problem.

The inflationary paradigm can resolve the flatness problem. During inflation the scale factor evolves as $a \propto t^p$ with $p > 1$, so $|\Omega_K|$ decreases in proportion to $|\Omega_K| \propto t^{2(1-p)}$. Provided the inflationary period is sufficiently long, the value of $|\Omega_K|$ at the end of inflation is extremely small. Even if $|\Omega_K|$ increases during the radiation and matter eras, it is possible to satisfy the bound (4.81).

Let us next proceed to the discussion of the horizon problem. A light traveling along the radial direction in the flat Universe obeys $ds^2 = 0$ in Eq. (4.1), i.e., $cdt = a(t)dr$. Integrating this relation from t_* to t , the comoving distance reads $d_c(t) = \int_{t_*}^t c/a(\tilde{t}) d\tilde{t}$. Then, the physical distance travelled by light (called the particle horizon) is given by

$$d_H(t) = a(t) d_c(t) = a(t) \int_{t_*}^t \frac{c d\tilde{t}}{a(\tilde{t})}. \quad (4.85)$$

In a decelerating Universe characterized by the evolution $a \propto t^p$ ($0 < p < 1$), taking the limit $t_* \rightarrow 0$ in Eq. (4.85) leads to

$$d_H(t) = \frac{ct}{1-p} = \frac{p}{1-p} cH^{-1}. \quad (4.86)$$

The quantity cH^{-1} , which determines the order of $d_H(t)$, is called the Hubble radius. From Eq. (2.10), the present Hubble radius is about $cH_0^{-1} \approx 10^{28}$ cm.

From Eq. (4.86), the causally connected region gets smaller as we go back to the past. For example, the particle horizon at the decoupling epoch ($z \simeq 1090$) should have been much smaller than its present value. However, the observed CMB photons traveling from the last scattering surface to us have almost the same intensity on any scales up to the present Hubble radius. This means that the causally connected region is much larger than the Hubble radius at the decoupling epoch in the real

Universe. This puzzle, which is called the horizon problem, can be addressed in the inflationary paradigm.

In the expanding Universe, the physical wavelength is the inverse of comoving wavenumber k multiplied by a , i.e., a/k , which grows very rapidly during inflation ($a \propto t^p$ with $p \gg 1$). On the other hand, for $p \gg 1$, the Hubble radius slowly grows as $H^{-1} \propto a^{1/p}$. Here and in the following, we use the natural unit $c = \hbar = k_B = 1$. At the onset of inflation, the region inside the Hubble radius ($a/k < H^{-1}$, i.e., $k/a > H$) is causally connected. During inflation, the physical wavelength a/k is stretched over the Hubble radius H^{-1} , so the causally connected region extends beyond H^{-1} . The Hubble radius crossing corresponds to

$$k = aH, \quad (4.87)$$

so the moment of crossing depends on k . For smaller k (i.e., for larger scales), the Hubble radius crossing occurs in the earlier epoch.

The inflationary period is followed by an epoch of the decelerated expansion described by the evolution $a \propto t^p$ ($0 < p < 1$), so the Hubble radius H^{-1} increases faster than the physical wavelength a/k . Then, the region with wavelength a/k crosses inside the Hubble radius again. For larger scales, this second Hubble radius crossing occurs at later cosmological epochs. For example, the mode entering the Hubble radius today corresponds to $a_0/k_0 = H_0^{-1} \approx 10^{28}$ cm. The wavelength that entered the Hubble radius at the CMB decoupling epoch is much smaller than a_0/k_0 . Both modes are causally connected because they were inside the Hubble radius at the onset of inflation.

The moment at which the mode with wavenumber k crossed the Hubble radius during inflation is given by $k = a_k H_k$, where the lower subscript k represents the instant at the first Hubble radius crossing. This can be regarded as the crossing of the comoving Hubble radius H^{-1}/a and the comoving wavelength k^{-1} [13]. The comoving Hubble radius decreases during inflation, but it increases during reheating, radiation-dominated, and matter-dominated epochs (see Fig. 4.2). The ratio $k/(a_0 H_0)$ can be expressed as

$$\frac{k}{a_0 H_0} = \frac{a_k H_k}{a_0 H_0} = e^{-\mathcal{N}(k)} \frac{a_{\text{end}}}{a_{\text{reh}}} \frac{a_{\text{reh}}}{a_{\text{eq}}} \frac{H_k}{H_{\text{eq}}} \frac{a_{\text{eq}} H_{\text{eq}}}{a_0 H_0}, \quad (4.88)$$

where the subscripts “end”, “reh”, “eq”, and “0” represent values at the end of inflation, at the end of reheating, at the radiation-matter equality, and at present, respectively. The quantity $\mathcal{N}(k)$ is called the number of e-foldings during inflation, which is defined by $\mathcal{N}(k) = \ln(a_{\text{end}}/a_k)$. Ignoring the contributions of dark energy and spatial curvature in Eq. (4.78) at $z = z_{\text{eq}}$, we can estimate H_{eq} as $H_{\text{eq}} = H_0 \sqrt{2\Omega_m^{(0)}} (1 + z_{\text{eq}})^{3/2}$, where $z_{\text{eq}} = a_0/a_{\text{eq}} - 1$ is given by Eq. (4.80). In terms of the unit of energy, the Hubble constant H_0 in Eq. (2.9) corresponds to $H_0 = 2.1332h \times 10^{-42}$ GeV. We also assume that the density ρ during reheating evolves

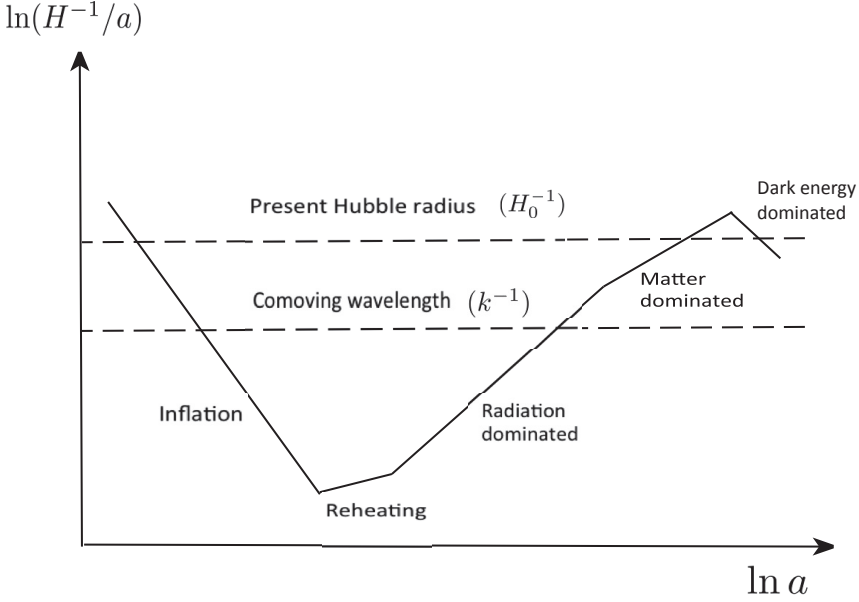


Fig. 4.2. Evolution of the comoving Hubble radius H^{-1}/a versus the scale factor a . Since H^{-1}/a decreases rapidly during inflation, it gets smaller than the comoving wavelength k^{-1} after the first Hubble radius crossing. During the radiation and matter eras, the comoving Hubble radius grows as $H^{-1}/a \propto a$ and $H^{-1}/a \propto a^{1/2}$, respectively, so the second Hubble radius crossing occurs in these epochs.

as $\rho \propto a^{-3}$. Then, from Eq. (4.88), it follows that

$$\mathcal{N}(k) = -\ln\left(\frac{k}{a_0 H_0}\right) + \frac{1}{3}\ln\left(\frac{\rho_{\text{reh}}}{\rho_{\text{end}}}\right) + \frac{1}{4}\ln\left(\frac{\rho_{\text{eq}}}{\rho_{\text{reh}}}\right) + \ln\left(\frac{H_k}{H_{\text{eq}}}\right) + \ln(219\Omega_m^{(0)}h). \quad (4.89)$$

Substituting the values $\Omega_m^{(0)} = 0.31$, $h = 0.68$, $z_{\text{eq}} = 3400$ into Eq. (4.89), the number of e-foldings is

$$\mathcal{N}(k) \simeq 68 - \ln\left(\frac{k}{a_0 H_0}\right) + \ln\left(\frac{H_k}{H_{\text{reh}}}\right) + \frac{1}{2}\ln\left(\frac{H_{\text{reh}}}{m_{\text{pl}}}\right) + \frac{1}{3}\ln\left(\frac{\rho_{\text{reh}}}{\rho_{\text{end}}}\right). \quad (4.90)$$

For smaller k the first Hubble radius crossing occurs earlier, so $\mathcal{N}(k)$ tends to be larger. If the reheating process occurs instantly and H_k is of the same order as H_{reh} , the largest scale observed in CMB measurements ($k \simeq a_0 H_0$) corresponds to $\mathcal{N}(k) = 63$ for $H_k = 10^{14}$ GeV. Depending on the detail of reheating, the value of $\mathcal{N}(k)$ is subject to change, but the typical number of e-foldings related to the observations of CMB temperature anisotropies is between 55 and 65. Provided the inflationary period is sufficiently long such that the number of e-foldings exceeds 65, the horizon problem can be resolved.

4.6.2. *Inflationary models and the scalar field dynamics*

The original model of inflation, which was based on a Higgs field appearing in Grand Unified Theories (GUT), was proposed by Sato [14], Kazanas [15], and Guth [16] in 1980. They showed that the vacuum energy of a Higgs field can lead to the cosmic acceleration during the process of the first-order phase transition. However, the bubble of vacuum collides after the end of inflation, which leads to a highly inhomogeneous Universe inconsistent with observations.

To address this problem of “old” inflation, a “new” inflationary scenario was proposed by Linde [17] and Albrecht and Steinhardt [18] in 1982. In this scenario, the second-order phase transition to a true vacuum leads to a slow-roll inflationary stage. The Higgs field, which is initially at a false vacuum, rolls down the potential with a decreasing temperature. Unlike old inflation, the Universe itself is inside the bubble, so the problem of the end of inflation can be avoided. However, there is a problem of the fine-tuning of initial conditions, i.e., the scalar field needs to stay at the false vacuum for a long time.

In 1983, Linde proposed a chaotic inflationary scenario in which the cosmic acceleration starts chaotically depending on initial conditions [19]. It is expected that there are regions in which large quantum fluctuations exist before the onset of inflation. If a scalar field ϕ evolves slowly in regions with large vacuum energies, the Universe exhibits the inflationary expansion. For the potential $V(\phi) = m^2\phi^2/2$, inflation occurs with the field value larger than the order of the Planck mass m_{pl} . After the field enters the region $\phi \lesssim 0.3m_{\text{pl}}$, its evolution tends to be faster with oscillations around the potential minimum at $\phi = 0$. During the oscillating stage of the scalar field, the energy density of ϕ is transferred to that of radiation. This process, which occurs after the end of inflation, is called reheating. After reheating, the Universe enters the radiation-dominated epoch with an initial temperature typically higher than 10^{20} K.

In addition to the said models, numerous inflationary models have been proposed so far. Most of them are based on the scalar field ϕ with its potential energy $V(\phi)$. Since the energy scale of inflation is much higher than that of the standard model of particle physics, the model building of inflation has usually been carried out by resorting to theories beyond the standard model, e.g., string theory and supergravity [20, 21]. In the following, we discuss general properties of inflation at the background level.

In GR, the action corresponding to the scalar field ϕ minimally coupled to gravity is given by

$$S = \int d^4x \sqrt{-g} \left(\frac{M_{\text{pl}}^2}{2} R + \mathcal{L}_\phi \right), \quad \mathcal{L}_\phi = -\frac{1}{2} g^{\mu\nu} \nabla_\mu \phi \nabla_\nu \phi - V(\phi), \quad (4.91)$$

where $M_{\text{pl}} = m_{\text{pl}}/\sqrt{8\pi}$ is the reduced Planck mass, and R is the Ricci scalar. The energy-momentum tensor $T_{\mu\nu}$ of the scalar field follows from the variation

of the matter action S_m given by Eq. (3.97), where the scalar-field action under consideration corresponds to $S_m = \int d^4x \sqrt{-g} \mathcal{L}_\phi$. On using Eq. (3.95), the scalar-field energy-momentum tensor yields

$$T_{\mu\nu} = -2 \frac{\delta \mathcal{L}_\phi}{\delta g^{\mu\nu}} + g_{\mu\nu} \mathcal{L}_\phi. \quad (4.92)$$

The mixed energy-momentum tensor $T_\mu^\lambda = g^{\lambda\nu} T_{\mu\nu}$ reads

$$T_\mu^\lambda = \nabla_\mu \phi \nabla^\lambda \phi + \delta_\mu^\lambda \left[-\frac{1}{2} \nabla_\alpha \phi \nabla^\alpha \phi - V(\phi) \right]. \quad (4.93)$$

Let us consider the flat FLRW background described by the line element $ds^2 = -dt^2 + a^2(t)(dx^2 + dy^2 + dz^2)$. In this case the energy-momentum tensor (4.93) reduces to $T_\mu^\lambda = \text{diag}(-\rho, P, P, P)$, where the density ρ and the pressure P are given, respectively, by

$$\rho = \frac{1}{2} \dot{\phi}^2 + V(\phi), \quad (4.94)$$

$$P = \frac{1}{2} \dot{\phi}^2 - V(\phi). \quad (4.95)$$

Neglecting the spatial curvature terms in Eqs. (4.15) and (4.19), it follows that

$$3M_{\text{pl}}^2 H^2 = \frac{1}{2} \dot{\phi}^2 + V, \quad (4.96)$$

$$2M_{\text{pl}}^2 \dot{H} = -\dot{\phi}^2. \quad (4.97)$$

Substituting Eqs. (4.94) and (4.95) into the continuity equation (4.20), we obtain

$$\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} = 0, \quad (4.98)$$

where $V_{,\phi} \equiv dV/d\phi$.

As long as the field ϕ (dubbed “inflaton”) evolves slowly along a nearly flat potential, inflation is driven by the potential energy $V(\phi)$. In the following, we employ the so-called slow-roll approximation characterized by the two conditions

$$\frac{1}{2} \dot{\phi}^2 \ll V, \quad |\ddot{\phi}| \ll |3H\dot{\phi}|, \quad (4.99)$$

under which Eqs. (4.96) and (4.98) reduce, respectively, to

$$3M_{\text{pl}}^2 H^2 \simeq V, \quad (4.100)$$

$$3H\dot{\phi} \simeq -V_{,\phi}. \quad (4.101)$$

Since the potential energy $V(\phi)$ slowly varies during inflation, the Hubble parameter H is nearly constant. To characterize the small variation of H , we define

the slow-roll parameter

$$\epsilon \equiv -\frac{\dot{H}}{H^2} \simeq \frac{3\dot{\phi}^2}{2V}, \quad (4.102)$$

which is much smaller than 1 during inflation. We also introduce other slow-roll parameters associated with slopes of the field potential:

$$\epsilon_V \equiv \frac{M_{\text{pl}}^2}{2} \left(\frac{V_{,\phi}}{V} \right)^2, \quad \eta_V \equiv \frac{M_{\text{pl}}^2 V_{,\phi\phi}}{V}. \quad (4.103)$$

Under the slow-roll approximation, these parameters are related to ϵ , as

$$\epsilon_V \simeq \epsilon, \quad \eta_V \simeq 2\epsilon - \frac{\dot{\epsilon}}{2H\epsilon}. \quad (4.104)$$

The conditions for realizing inflation correspond to $\{\epsilon_V, |\eta_V|\} \ll 1$. Inflation ends when the parameters ϵ_V and $|\eta_V|$ grow to the order of 1.

To quantify the amount of inflation, we introduce the number of e-foldings, as

$$\mathcal{N} = \ln \frac{a(t_{\text{end}})}{a(t)}, \quad (4.105)$$

where $a(t)$ and $a(t_{\text{end}})$ are the scale factors at time t during inflation and at time t_{end} corresponding to the end of inflation. Taking the time derivative of Eq. (4.105), it follows that $d\mathcal{N}/dt = -H$. Integrating this relation back from t_{end} to t , we obtain

$$\mathcal{N} = - \int_{t_{\text{end}}}^t H(\tilde{t}) d\tilde{t} \simeq \frac{1}{M_{\text{pl}}^2} \int_{\phi_{\text{end}}}^{\phi} \frac{V}{V_{,\tilde{\phi}}} d\tilde{\phi}, \quad (4.106)$$

where we used Eqs. (4.100) and (4.101).

For example, let us first consider the potential of chaotic inflation given by [19]

$$V(\phi) = \frac{\lambda}{n} \phi^n, \quad (4.107)$$

where n and λ are positive constants. This potential is schematically plotted in the left panel of Fig. 4.3. Estimating the field value ϕ_{end} at the end of inflation under the condition $\epsilon_V(\phi_{\text{end}}) = 1$, it follows that $\phi_{\text{end}} = nM_{\text{pl}}/\sqrt{2}$. For $n = 2$ and $n = 4$, we have $\phi_{\text{end}} = \sqrt{2}M_{\text{pl}}$ and $\phi_{\text{end}} = 2\sqrt{2}M_{\text{pl}}$, respectively. From Eq. (4.106), the field value ϕ is related to the number of e-foldings, as

$$\phi(\mathcal{N}) \simeq \sqrt{2n \left(\mathcal{N} + \frac{n}{4} \right)} M_{\text{pl}}. \quad (4.108)$$

For $n = 2$ and $n = 4$ with $\mathcal{N} = 60$, $\phi = 15.6M_{\text{pl}}$ and $\phi = 22.1M_{\text{pl}}$, respectively. The cosmic acceleration commences from the field value larger than M_{pl} in chaotic inflation. The field variation $\Delta\phi$ during inflation is larger than the order of M_{pl} .

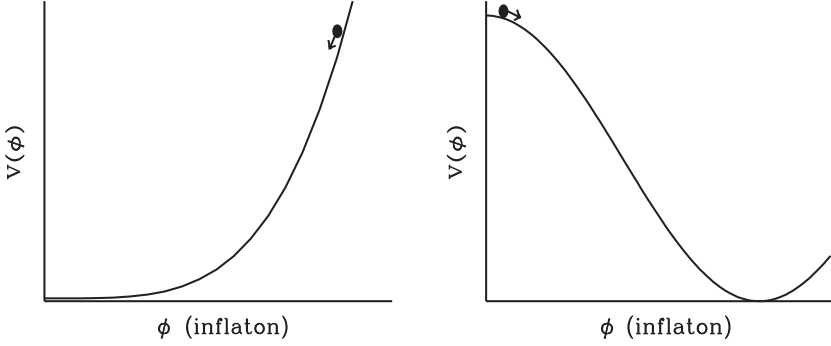


Fig. 4.3. Scalar-field potentials of chaotic inflation (left) and natural inflation (right).

There are models in which the second derivative $V_{,\phi\phi}$ changes its sign. As an example, we consider the natural inflation model based on the Pseudo–Nambu–Goldstone–Boson (PNGB) boson [22]. The potential in this model is given by

$$V(\phi) = V_0 \left[1 + \cos\left(\frac{\phi}{f}\right) \right], \quad (4.109)$$

where V_0 and f are constants (see the right panel of Fig. 4.3). From the condition $\epsilon_V(\phi_{\text{end}}) = 1$ the field value at the end of inflation satisfies $\tan^2[\phi_{\text{end}}/(2f)] = 2(f/M_{\text{pl}})^2$, e.g., $\phi_{\text{end}} = 2.86f$ for $f = \sqrt{8\pi}M_{\text{pl}}$. The number of e-foldings corresponding to the field value ϕ is

$$\mathcal{N} = \frac{2f^2}{M_{\text{pl}}^2} \ln \left[\frac{\sin(\phi_{\text{end}}/(2f))}{\sin(\phi/(2f))} \right]. \quad (4.110)$$

For $f = \sqrt{8\pi}M_{\text{pl}}$ and $\mathcal{N} = 60$, we have $\phi = 0.61f$. In this case the curvature of the potential is negative ($V_{,\phi\phi} < 0$) in the early stage of inflation, so the slow-roll parameter η_V is negative. This property affects the primordial power spectrum of curvature perturbations generated during inflation. For smaller f , the inflaton field needs to be closer to 0 to lead to a sufficient amount of inflation.

It is also possible to drive inflation in the presence of the quadratic Ricci scalar term R^2 besides the Einstein–Hilbert term R . The action of this model, which is called the Starobinsky inflation [23], is given by

$$S = \frac{M_{\text{pl}}^2}{2} \int d^4x \sqrt{-g} f(R), \quad f(R) = R + \frac{R^2}{6M^2}, \quad (4.111)$$

where M is a constant having a dimension of mass. As we will see in Sec. 11.2, the action (4.111) can be transformed to the “Einstein-frame” action (4.91) under a so-called conformal transformation of the metric $g_{\mu\nu}$. In the Einstein frame, a scalar degree of freedom $\phi = \sqrt{3/2}M_{\text{pl}} \ln \partial f / \partial R$ explicitly arises from the gravity

sector with the field potential $V(\phi) = (M_{\text{pl}}^2/2)e^{-2\sqrt{6}\phi/(3M_{\text{pl}})}[R(\partial f/\partial R) - f]$, see Eqs. (11.80) and (11.81).

For the Starobinsky model (4.111), the potential in the Einstein frame yields

$$V(\phi) = \frac{3}{4}M^2M_{\text{pl}}^2 \left(1 - e^{-\sqrt{2/3}\phi/M_{\text{pl}}}\right)^2, \quad (4.112)$$

where $\phi = \sqrt{3/2}M_{\text{pl}}\ln[1 + R/(3M^2)]$. For $\phi \gg M_{\text{pl}}$ the potential (4.112) is nearly constant, so the slow-roll inflation is realized in this regime. After the field enters the regime $\phi \ll M_{\text{pl}}$, the potential is approximately given by $V(\phi) \simeq M^2\phi^2/2$. Hence the Universe finally enters a reheating stage with the oscillation of ϕ . Since the slow-roll parameter ϵ_V is given by $\epsilon_V = (4/3)[e^{\sqrt{6}\phi/(3M_{\text{pl}})} - 1]^{-2}$, the field value ϕ_{end} at the end of inflation is known as $\phi_{\text{end}} = 0.94M_{\text{pl}}$ from the condition $\epsilon_V(\phi_{\text{end}}) = 1$. Since inflation occurs for ϕ larger than M_{pl} , the number of e-foldings (4.106) can be estimated as

$$\mathcal{N} \simeq \frac{3}{4}e^{\sqrt{6}\phi/(3M_{\text{pl}})}, \quad (4.113)$$

which exceeds $\mathcal{N} = 65$ for $\phi > 5.46M_{\text{pl}}$. In the regime $\phi \gg M_{\text{pl}}$, the two slow-roll parameters ϵ_V and η_V are approximately given by

$$\epsilon_V \simeq \frac{4}{3}e^{-2\sqrt{6}\phi/(3M_{\text{pl}})} \simeq \frac{3}{4\mathcal{N}^2}, \quad (4.114)$$

$$\eta_V \simeq -\frac{4}{3}e^{-\sqrt{6}\phi/(3M_{\text{pl}})} \simeq -\frac{1}{\mathcal{N}}, \quad (4.115)$$

which will be used for the computation of the scalar and tensor power spectra in Sec. 6.8.

The observational data of CMB temperature anisotropies allows one to distinguish between different inflationary models explained above.

4.7. Reheating

After the end of inflation, the Universe enters the reheating epoch in which the inflaton field ϕ decays to other particles. To study the dynamics of reheating, we consider the field potential of chaotic inflation:

$$V(\phi) = \frac{1}{2}m_\phi^2\phi^2, \quad (4.116)$$

where m_ϕ is a constant having a dimension of mass. During reheating, the field oscillates rapidly around the potential minimum ($\phi = 0$). We focus on the reheating dynamics for the potential (4.116), but we can also perform a similar analysis for other inflaton potentials by expanding them around their potential minima.

In the early stage of reheating where the density of produced particles is much smaller than that of inflaton, the equations of motion on the flat FLRW background are given by Eqs. (4.96) and (4.98), i.e.,

$$3M_{\text{pl}}^2 H^2 = \frac{1}{2}\dot{\phi}^2 + \frac{1}{2}m_\phi^2 \phi^2, \quad (4.117)$$

$$\ddot{\phi} + 3H\dot{\phi} + m_\phi^2 \phi = 0. \quad (4.118)$$

As we will see in Sec. 6.8, the inflaton mass is constrained to be $m_\phi \simeq 10^{13}$ GeV from the amplitude of observed CMB temperature anisotropies. During inflation m_ϕ is smaller than H , but the Hubble parameter drops below m_ϕ around the onset of reheating. On using the approximation $m_\phi^2 \gg \{H^2, |\dot{H}|\}$ during reheating and redefining a new field $\tilde{\phi} = a^{3/2}\phi$, Eq. (4.118) reduces to $\ddot{\tilde{\phi}} + m_\phi^2 \tilde{\phi} \simeq 0$. The solution to this equation is given by $\tilde{\phi}(t) = a^{3/2}\phi(t) = \tilde{\phi}_0 \sin(m_\phi t)$, where $\tilde{\phi}_0$ is a constant. Taking the time average over oscillations, the virial theorem $\langle \dot{\phi}^2/2 \rangle = \langle m_\phi^2 \phi^2/2 \rangle = m_\phi^2 \tilde{\phi}_0^2/(4a^3)$ holds in Eq. (4.117). Then, we obtain the integrated solutions

$$a(t) = a_i \left(\frac{t}{t_i} \right)^{2/3}, \quad (4.119)$$

$$\phi(t) = \phi_0(t) \sin(m_\phi t), \quad \phi_0(t) = \sqrt{\frac{8}{3}} \frac{M_{\text{pl}}}{m_\phi t}, \quad (4.120)$$

where a_i is the value of a at the onset of reheating ($t = t_i$). The evolution of a for the massive scalar field is the same as that in the matter-dominated epoch.

Let us consider the case in which the inflaton field ϕ decays to a fermionic particle φ with mass m_φ and a bosonic particle χ with mass m_χ [24, 25]. The interacting Lagrangian in such a system is given by

$$\mathcal{L}_{\text{int}} = -f\phi\bar{\varphi}\varphi - \sigma\phi\chi^2, \quad (4.121)$$

where f is a dimensionless constant, and σ is a constant having a dimension of mass. In what follows, we employ a so-called Born approximation under which the inflaton field is treated as a classical external field. As long as the condition $m_\phi \gg H$ holds during reheating, we can neglect the effect of cosmic expansion on the creation rate of particles. We also assume that the effective mass of produced particles is much smaller than m_ϕ . Using the first-order perturbation theory for the couplings f and σ , the production rates of particles per unit volume and per time are given, respectively, by [26]

$$n_{\bar{\varphi}\varphi} = \frac{f^2}{16\pi} (\phi_0 m_\phi)^2, \quad n_{\chi\chi} = \frac{1}{16\pi} (\sigma \phi_0)^2. \quad (4.122)$$

The time average of the inflaton energy density is $\langle \rho_\phi \rangle = m_\phi^2 \phi_0^2/2$. Using the fact that the average energy per particle is of the order of m_ϕ , the decay rates of ϕ to φ

and χ reduce, respectively, to

$$\Gamma_\varphi = \frac{n_{\bar{\varphi}\varphi} m_\phi}{\langle \rho_\phi \rangle} = \frac{f^2 m_\phi}{8\pi}, \quad \Gamma_\chi = \frac{n_{\chi\chi} m_\phi}{\langle \rho_\phi \rangle} = \frac{\sigma^2}{8\pi m_\phi}, \quad (4.123)$$

where the total decay rate is $\Gamma = \Gamma_\varphi + \Gamma_\chi$.

To reflect the decay of particles from the field ϕ to radiation (energy density ρ_r), we need to take into account the term $\Gamma\langle\rho_\phi\rangle$ to the radiation continuity equation $\dot{\rho}_r + 4H\rho_r = 0$, i.e.,

$$\dot{\rho}_r + 4H\rho_r = \Gamma\langle\rho_\phi\rangle. \quad (4.124)$$

The field ϕ with mass m_ϕ behaves as a non-relativistic particle during the oscillating phase of inflaton. If there is no decay to radiation, the average energy density $\langle\rho_\phi\rangle$ of inflaton obeys the continuity equation $\langle\dot{\rho}_\phi\rangle + 3H\langle\rho_\phi\rangle = 0$. Now the field ϕ decays to radiation, so the total energy conservation of ϕ and radiation leads to

$$\langle\dot{\rho}_\phi\rangle + 3H\langle\rho_\phi\rangle = -\Gamma\langle\rho_\phi\rangle. \quad (4.125)$$

Differentiating $\rho_\phi = \dot{\phi}^2/2 + V(\phi)$ with respect to t and taking the time average, Eq. (4.125) reduces to

$$\ddot{\phi} + (3H + \Gamma)\dot{\phi} + m_\phi^2\phi = 0. \quad (4.126)$$

We can integrate Eq. (4.125) to give

$$\langle\rho_\phi\rangle = \rho_\phi^{(i)} \left(\frac{a}{a_i}\right)^{-3} e^{-\Gamma(t-t_i)}, \quad (4.127)$$

where $\rho_\phi^{(i)}$ is the value of $\langle\rho_\phi\rangle$ at $t = t_i$. In the early stage of reheating in which the condition $\Gamma(t - t_i) \ll 1$ is satisfied, the inflaton energy density decreases as $\langle\rho_\phi\rangle \propto a^{-3}$. Around the time $t \gtrsim t_i + 1/\Gamma$, the exponential term in Eq. (4.127) starts to cause a rapid decrease of $\langle\rho_\phi\rangle$. Substituting the relation $\langle\rho_\phi\rangle \simeq \rho_\phi^{(i)} (a/a_i)^{-3}$ into Eq. (4.124) for $t \lesssim t_i + 1/\Gamma$, we obtain the integrated solution

$$\rho_r(t) = \frac{3\Gamma\rho_\phi^{(i)}t_i^2}{5t} \left[1 - \left(\frac{t}{t_i}\right)^{-5/3} \right], \quad (4.128)$$

where we used the initial condition $\rho_r(t_i) = 0$ and the fact that $a \propto t^{2/3}$ for $t_i < t \lesssim t_i + 1/\Gamma$.

The radiation density (4.128) grows from $t = t_i$ and then reaches a maximum value at $t \simeq 1.8t_i$. For $t > 1.8t_i$, the radiation density decreases as $\rho_r \propto t^{-1} \propto a^{-3/2}$ up to the time $t \simeq 1/\Gamma$ (under the condition $t_i \ll 1/\Gamma$). Even if $\rho_r < \rho_\phi$ at $t \simeq 1.8t_i$, ρ_r decreases more slowly than ρ_ϕ for $t > 1.8t_i$. Then, ρ_r catches up with ρ_ϕ around the time $t = t_{\text{reh}} \equiv 1/\Gamma$. For $t > t_{\text{reh}}$, $\langle\rho_\phi\rangle$ exponentially decreases in time, whereas

ρ_r evolves as $\rho_r \propto a^{-4}$. On using Eq. (4.128), the radiation density at time $t = t_{\text{reh}}$ can be estimated as

$$\rho_r(t_{\text{reh}}) \simeq \frac{3}{5}\Gamma^2 \rho_\phi^{(i)} t_i^2 \simeq \frac{3\Gamma^2 \rho_\phi^{(i)}}{5H_i^2} \simeq \frac{9}{5}\Gamma^2 M_{\text{pl}}^2, \quad (4.129)$$

where we used $t_i \simeq 1/H_i$ and $\rho_\phi^{(i)} = 3M_{\text{pl}}^2 H_i^2$.

From Eq. (4.38) the radiation density at the onset of the radiation era (denoted by the reheating temperature T_{reh}) is given by $\rho_r(t_{\text{reh}}) = \pi^2 g_* T_{\text{reh}}^4/30$ (where we consider bosonic particles, but the estimation is similar for fermions). The relativistic degrees of freedom g_* can be around 100~200 in the very early Universe. Taking the value $g_* = 100$ and solving the equation $(9/5)\Gamma^2 M_{\text{pl}}^2 = \pi^2 g_* T_{\text{reh}}^4/30$ for T_{reh} , it follows that

$$T_{\text{reh}} \simeq 0.5\sqrt{\Gamma M_{\text{pl}}}. \quad (4.130)$$

If we consider the decay of inflaton to fermions φ with the coupling $f = 10^{-6}$ in Eq. (4.123), the reheating temperature can be estimated as $T_{\text{reh}} = 5 \times 10^8$ GeV. If massive particles like gravitinos (superpartner of gravitons in the context of supersymmetric theories) are overproduced during reheating, this can prevent the successful cosmic expansion history of the Universe. To avoid the overproduction of gravitinos, the reheating temperature is constrained to be $T_{\text{reh}} \lesssim 10^9$ GeV [27], whose upper limit corresponds to 10^{22} K. For $t > 1/\Gamma$, the Universe enters the radiation-dominated epoch.

The above discussion is based on the perturbation theory with perturbative decays rates (4.123). If there exists a four-point interaction term $g^2 \phi^2 \chi^2/2$, a non-perturbative particle production called preheating occurs before the perturbative decay discussed above [28, 29]. During preheating, χ particles can be efficiently produced by a parametric resonance. It is known, however, that existence of the preheating stage does not significantly affect the estimation of the reheating temperature (4.130).

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Chapter 5

Observational Evidence of Dark Energy at the Background Level

In 1998, the first direct observational evidence of the late-time cosmic acceleration was reported from the observations of supernovae type Ia (SN Ia). Even before this discovery, there were several pieces of evidence of a “missing matter” problem — such as those from the age of the Universe and number counts of faint galaxies. In this chapter, we first review the problems of cosmic age and number counts of galaxies already known in the early 1990s. We then proceed to describe how the cosmic acceleration was discovered from the SN Ia measurements.

After 1998, the existence of dark energy responsible for the cosmic acceleration was also confirmed by other independent observations such as CMB, BAO, and galaxy clusterings. Since they are associated with the development of inhomogeneities, the knowledge of cosmological perturbation theory is essential for us to understand how the properties of dark energy are constrained from those observations. In this chapter we focus on observational evidence of dark energy at the background level and then in Chap. 8 we will discuss how the observations related to the growth of inhomogeneities place constraints on dark energy.

5.1. Age of the Universe

In the 1990s, there was a problem regarding the age of the Universe (t_0) compared to the age of oldest stellar populations (t_s). For the Universe dominated by non-relativistic matter (dubbed the Einstein de Sitter model), the measurements of globular clusters showed that t_s is usually larger than t_0 . For instance, the age of the globular cluster M4 was constrained as $t_s = 12.7 \pm 0.7$ Gyr by employing the cooling sequence method of white dwarfs [1]. Jimenez *et al.* constrained the age of globular clusters in the Milky Way as $t_s = 13.5 \pm 2$ Gyr by using a distance-independent method [2]. As we will see below, the age of the Universe in the Einstein de Sitter model is smaller than 10 Gyr, so in this case there is an inconsistency: $t_0 < t_s$. This problem can be resolved by assuming the existence of dark energy.

We compute the age of the FLRW Universe by taking into account three energy components: radiation ($w_r = 1/3$), non-relativistic matter ($w_m = 0$), and the cosmological constant ($w_{\text{DE}} = -1$). In principle we can consider other forms of dark energy whose equation of state is different from -1 , but the qualitative estimation of t_0 is not very different from the one given below. From Eq. (4.78) the Hubble parameter at the redshift z reads

$$H^2 = H_0^2 [\Omega_r^{(0)}(1+z)^4 + \Omega_m^{(0)}(1+z)^3 + \Omega_{\text{DE}}^{(0)} + \Omega_{\mathcal{K}}^{(0)}(1+z)^2]. \quad (5.1)$$

Setting $z = 0$ in Eq. (5.1), it follows that

$$\Omega_r^{(0)} + \Omega_m^{(0)} + \Omega_{\text{DE}}^{(0)} + \Omega_{\mathcal{K}}^{(0)} = 1. \quad (5.2)$$

Taking the time derivative of the relation $1+z = a_0/a$, we obtain $dt/dz = -1/[(1+z)H]$. Then, the age of the Universe can be computed as

$$t_0 = \int_0^{t_0} dt = \int_0^\infty \frac{dz}{(1+z)H} = \frac{1}{H_0} \int_1^\infty \frac{dx}{x[\Omega_r^{(0)}x^4 + \Omega_m^{(0)}x^3 + \Omega_{\text{DE}}^{(0)} + \Omega_{\mathcal{K}}^{(0)}x^2]^{1/2}}, \quad (5.3)$$

where $x \equiv 1+z$. The main contributions to the integral (5.3) come from those in the low redshifts ($x \lesssim 10$). Since $\Omega_r^{(0)}$ is constrained to be much smaller than 1 (at most of the order of 10^{-4}), we can ignore the contribution of radiation in Eq. (5.3) for the evaluation of t_0 .

We begin with the case in which the cosmological constant is absent ($\Omega_{\text{DE}}^{(0)} = 0$). In the flat Universe characterized by $\Omega_{\mathcal{K}}^{(0)} = 0$, we have $\Omega_m^{(0)} = 1$ and hence the integral (5.3) reduces to

$$t_0 = \frac{1}{H_0} \int_1^\infty \frac{dx}{x^{5/2}} = \frac{2}{3H_0}. \quad (5.4)$$

From Eq. (2.9), the inverse of the Hubble constant is given by $H_0^{-1} = 9.776h^{-1}$ Gyr. On using the bound $0.64 < h < 0.80$ derived from the Hubble Space Telescope Key Project [3], the age (5.4) corresponds to $t_0 = 8 \sim 10$ Gyr. Since this is smaller than the age of oldest globular clusters, the flat Universe without the cosmological constant is plagued by the age problem.

Let us consider the open Universe ($\Omega_{\mathcal{K}}^{(0)} > 0$) without the cosmological constant ($\Omega_{\text{DE}}^{(0)} = 0$). In this case the non-relativistic matter density is given by $\Omega_m^{(0)} = 1 - \Omega_{\mathcal{K}}^{(0)} < 1$. From Eq. (5.3), the age of the Universe yields

$$\begin{aligned} t_0 &= \frac{1}{H_0} \int_1^\infty \frac{dx}{x^2[\Omega_m^{(0)}x + 1 - \Omega_m^{(0)}]^{1/2}} \\ &= \frac{1}{H_0} \left[\frac{1}{1 - \Omega_m^{(0)}} + \frac{\Omega_m^{(0)}}{2(1 - \Omega_m^{(0)})^{3/2}} \ln \left(\frac{1 - \sqrt{1 - \Omega_m^{(0)}}}{1 + \sqrt{1 - \Omega_m^{(0)}}} \right) \right]. \end{aligned} \quad (5.5)$$

In the limit that $\Omega_m^{(0)} \rightarrow 0$, we have $t_0 \rightarrow 1/H_0$, whereas, for $\Omega_m^{(0)} \rightarrow 1$, $t_0 \rightarrow 2/(3H_0)$. For smaller $\Omega_m^{(0)}$, the cosmic age is larger than that in the flat model discussed above. As the amount of matter decreases, it takes longer for gravitational interactions to slow down the Hubble expansion rate to its present value. Since $\Omega_{\mathcal{K}}^{(0)}$ is close to 0 from the observations of CMB temperature anisotropies [see Eq. (4.81)], the age of the Universe does not exceed the oldest stellar age.

This cosmic age problem can be resolved in the presence of the cosmological constant ($\Omega_{\text{DE}}^{(0)} > 0$). In the flat Universe ($\Omega_{\mathcal{K}}^{(0)} = 0$) satisfying the relation $\Omega_m^{(0)} + \Omega_{\text{DE}}^{(0)} = 1$, the integral (5.3) reduces to

$$t_0 = \frac{1}{H_0} \int_1^\infty \frac{dx}{x\sqrt{\Omega_m^{(0)}x^3 + 1 - \Omega_m^{(0)}}} = \frac{2}{3H_0\sqrt{1 - \Omega_m^{(0)}}} \ln \left(\frac{1 + \sqrt{1 - \Omega_m^{(0)}}}{\sqrt{\Omega_m^{(0)}}} \right). \quad (5.6)$$

For $\Omega_m^{(0)} \rightarrow 0$ we have $t_0 \rightarrow \infty$, whereas, for $\Omega_m^{(0)} \rightarrow 1$, $t_0 \rightarrow 2/(3H_0)$. With the decrease of $\Omega_m^{(0)}$, the age of the Universe gets larger. For $\Omega_m^{(0)} = 0.32$ and $h = 0.67$, it follows that $t_0 = 0.946H_0^{-1} = 13.8 \text{ Gyr}$, which is larger than the age of the oldest stellar populations. Hence the existence of dark energy addresses the cosmic age problem. Even though this fact was known before the early 1990s, the existence of the cosmological constant was still doubted due to the lack of direct evidence of the accelerating Universe.

5.2. Number counts of faint galaxies

In the 1980s, there were a number of deep surveys for counting the number of faint galaxies. In particular, the CCD number counts of faint galaxies reported by Tyson [4] and Broadhurst *et al.* [5] provided useful information about the matter content of the Universe at low redshifts. As we explained in Sec. 5.1, the cosmic age gets larger in the presence of the cosmological constant Λ . Provided that the density of galaxies stays nearly constant in the past and today, the existence of Λ gives rise to a larger observed volume of galaxies due to the increase of the cosmic age. As a result, the number of faint galaxies observed by us should increase for larger Λ .

In 1990, Fukugita *et al.* [6] found that the model with $\Omega_m^{(0)} \gtrsim 0.5$ (where $\Omega_m^{(0)}$ is the density parameter of non-relativistic matter) is strongly disfavored from the observational data of Tyson by assuming a standard evolution model of galaxies. Moreover, they showed that the best-fit is achieved in the presence of the cosmological constant with $\Omega_{\text{DE}}^{(0)}$ between 0.5 and 1.

In Fig. 5.1, the number count n of galaxies is plotted as a function of the apparent magnitude m (denoted as B_J in the figure, see Sec. 5.3 for the definition of the apparent magnitude). The theoretical curve (a) corresponds to a flat Universe without the cosmological constant (i.e., the Einstein de Sitter Universe), in which case the model does not fit the data in the region of high m . The case (b) shows

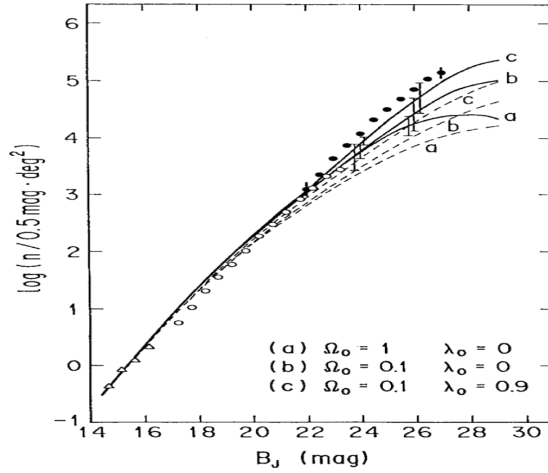


Fig. 5.1. Number counts of galaxies as a function of the apparent magnitude m in the so-called B_J band. The data points are taken from Tyson [4] for $22 \leq B_J \leq 27$ mag (CCD) and $17 \leq B_J \leq 23$ mag (photographic), and from Kirshner *et al.* [7] for $B_J \leq 17$ mag. Each theoretical curve corresponds to (a) a flat Universe with $\Omega_m^{(0)} = 1$ and $\Omega_{DE}^{(0)} = 0$, (b) an open Universe with $\Omega_m^{(0)} = 0.1$ and $\Omega_{DE}^{(0)} = 0$, and (c) a flat Universe with $\Omega_m^{(0)} = 0.1$ and $\Omega_{DE}^{(0)} = 0.9$. The cosmological constant Λ is assumed for the origin of dark energy. Dashed curves represent the corresponding no-evolution model of galaxies for each case. Reproduced from Ref. [6].

the model prediction for an open Universe without Λ ($\Omega_m^{(0)} = 0.1$ and $\Omega_{DE}^{(0)} = 0.9$), which gives rise to larger values of n relative to the case (a). However, this model does not fit the data very well. The curve (c) corresponds to a flat Universe with $\Omega_m^{(0)} = 0.1$ and $\Omega_{DE}^{(0)} = 0.9$, in which case the model shows a better fit to the data compared to the cases (a) and (b).

Thus the existence of the cosmological constant can be suggested from the data of Tyson. The number counting method used by Fukugita *et al.* did not take into account uncertainties for the evolution model of galaxies (like possible changes of galaxy density and luminosity during the process of evolution), so it was anticipated that there may be a better galaxy evolution model fitting the data better even without Λ . In this sense, the result mentioned above was not regarded as a smoking gun for the existence of dark energy. However, along with the cosmic age problem, the number counts of faint galaxies provided important signatures for the inconsistency of models without dark energy. In fact, as we will see in Sec. 5.3, the fact that dark energy dominates over non-relativistic matter in the present Universe was confirmed by SN Ia measurements in the late 1990s.

5.3. Supernovae type Ia

The first direct evidence of late-time cosmic acceleration was found by the distance measurements of SN Ia in 1998 [8, 9]. In what follows, we first discuss how the luminosity distance used in SN Ia measurements is related to the expansion rate of

the Universe. We then proceed to the explanation of how the accelerated expansion was discovered.

5.3.1. *Luminosity distance*

Let us consider a bright object with an absolute luminosity L_s . Here, the absolute luminosity is defined as the energy emitted from the source per unit time. The flux $\mathcal{F}$ observed on Earth corresponds to the energy observed per unit time and unit area. We define the luminosity distance d_L , as

$$d_L^2 = \frac{L_s}{4\pi\mathcal{F}}. \quad (5.7)$$

We use the metric (4.4) to study the propagation of a light on the FLRW background. Suppose that the observer is located at $\chi = 0$. If the light with an energy ΔE_1 is emitted from the source located at distance χ (at redshift z) with a time period Δt_1 , then the absolute luminosity of the source is given by $L_s = \Delta E_1/\Delta t_1$. If the observer receives the same light as an energy ΔE_0 with a time period Δt_0 , then the apparent luminosity becomes $L_0 = \Delta E_0/\Delta t_0$. Since the energy of photons is inversely proportional to its wavelength, we have the following relation

$$\frac{\Delta E_1}{\Delta E_0} = \frac{\lambda_0}{\lambda_1} = 1 + z, \quad (5.8)$$

where λ_1 and λ_0 are wavelengths emitted from the source and detected by the observer, respectively. Since the speed of light is given by $c = \lambda_1/\Delta t_1 = \lambda_0/\Delta t_0$, it follows that $\Delta t_0/\Delta t_1 = 1 + z$. Then, the ratio between L_s and L_0 yields

$$\frac{L_s}{L_0} = (1 + z)^2. \quad (5.9)$$

Since the physical distance between source and observer is $a_0 f_K(\chi)$, where a_0 is the scale factor today, the observed flux is given by

$$\mathcal{F} = \frac{L_0}{4\pi[a_0 f_K(\chi)]^2}. \quad (5.10)$$

Substituting Eq. (5.10) into Eq. (5.7) and using Eq. (5.9), it follows that

$$d_L = a_0 f_K(\chi)(1 + z). \quad (5.11)$$

From Eq. (4.8), the comoving distance between source and observer can be expressed as

$$\chi = \frac{1}{a_0 H_0} \int_0^z \frac{d\tilde{z}}{E(\tilde{z})}, \quad (5.12)$$

where $E(z) = H(z)/H_0$. Here and in the following we use the unit $c = 1$. From Eq. (4.5) and the definition $\Omega_K^{(0)} = -\mathcal{K}/(a_0^2 H_0^2)$, the luminosity distance (5.11)

reads

$$d_L(z) = \frac{1+z}{H_0 \sqrt{\Omega_{\mathcal{K}}^{(0)}}} \sinh \left(\sqrt{\Omega_{\mathcal{K}}^{(0)}} \int_0^z \frac{d\tilde{z}}{E(\tilde{z})} \right). \quad (5.13)$$

This shows that $d_L(z)$ is directly related to the Hubble expansion rate $H(z)$. If the luminosity distance is measured observationally, it is possible to place constraints on the expansion rate and matter contents in the Universe.

5.3.2. *Discovery of the cosmic acceleration*

The luminosity distance d_L is known by measuring the difference between an absolute magnitude M of the source and an observed apparent magnitude m on Earth. The astronomical definition of the apparent magnitude is that a star with $m_1 = 1$ is 100 times as bright as another star with $m_2 = 6$. The observed brightness depends on the flux $\mathcal{F}$. If there are two stars observed by apparent magnitudes m_1 and m_2 with corresponding fluxes $\mathcal{F}_1$ and $\mathcal{F}_2$, the following relation holds:

$$m_1 - m_2 = -\frac{5}{2} \log_{10} \left(\frac{\mathcal{F}_1}{\mathcal{F}_2} \right). \quad (5.14)$$

Suppose that the absolute luminosities L_s of two stars are the same as each other. On using the relation (5.7), it follows that

$$m_1 - m_2 = 5 \log_{10} \left(\frac{d_{L_1}}{d_{L_2}} \right), \quad (5.15)$$

where d_{L_1}, d_{L_2} are luminosity distances to stars with apparent magnitudes m_1, m_2 , respectively. If $m_1 = 1$ and $m_2 = 6$, for example, we have $d_{L_2} = 10d_{L_1}$. For the star with a larger luminosity distance d_L , the apparent magnitude m gets larger.

We define the absolute magnitude M of a star with the luminosity distance d_L according to the relation

$$m - M = 5 \log_{10} \left(\frac{d_L}{10 \text{ pc}} \right), \quad (5.16)$$

where m is the observed apparent magnitude. This means that the absolute magnitude corresponds to the apparent magnitude of the object at the distance of exactly 10 pc from the observer. If we consider two stars with the same absolute magnitude M , then the relation (5.16) is consistent with Eq. (5.15).

The supernova explosion is a very bright astronomical phenomenon that occurs at the end of the stellar evolution process. One can classify the types of supernovae depending on what kinds of spectral lines exist. The SN Ia have the spectral line of silicon but without the spectral line of hydrogen. The type Ia supernovae explosion occurs when the mass of a white dwarf in a binary system exceeds a Chandrasekhar mass.

At the peak of brightness, the SN Ia have a nearly constant absolute magnitude ($M \simeq -19$), so it can be treated as a standard candle. By measuring apparent magnitudes m at many different redshifts z , the luminosity distance d_L is known as a function of z . Theoretical values of $d_L(z)$ are different depending on whether dark energy is present or not, so we can probe the existence of dark energy from the observational data of SN Ia.

The observed SN Ia data were in the redshift regime $z \lesssim 3$, so it is a good approximation to ignore the contribution of radiation in Eq. (5.1). In the flat Universe, the normalized Hubble parameter squared is given by $E^2(z) \simeq (1 - \Omega_{\text{DE}}^{(0)})(1+z)^3 + \Omega_{\text{DE}}^{(0)}$ from Eqs. (5.1) and (5.2). Then, the luminosity distance (5.13) yields

$$d_L(z) = \frac{1+z}{H_0} \int_0^z \frac{d\tilde{z}}{E(\tilde{z})} = \frac{1+z}{H_0} \int_0^z \frac{d\tilde{z}}{[(1 - \Omega_{\text{DE}}^{(0)})(1+\tilde{z})^3 + \Omega_{\text{DE}}^{(0)}]^{1/2}}. \quad (5.17)$$

In the regime $z \ll 1$, we have the approximate relation $E(z) \simeq 1 + 3z(1 - \Omega_{\text{DE}}^{(0)})/2$. For larger $\Omega_{\text{DE}}^{(0)}$, the denominator inside the integral of (5.17) gets smaller, so the luminosity distance increases. The numerical integration of Eq. (5.17) shows that, for increasing $\Omega_{\text{DE}}^{(0)}$, $d_L(z)$ gets larger for $z \gtrsim 1$ as well.

In Fig. 5.2, theoretical curves of $d_L(z)$ are plotted for the flat Λ CDM model in the redshift regime $0 \leq z \leq 2$ with three different values of $\Omega_{\text{DE}}^{(0)}$. As mentioned above, the luminosity distance increases for larger $\Omega_{\text{DE}}^{(0)}$. This reflects the fact that, in the accelerating Universe, the SN Ia look fainter compared to the decelerating

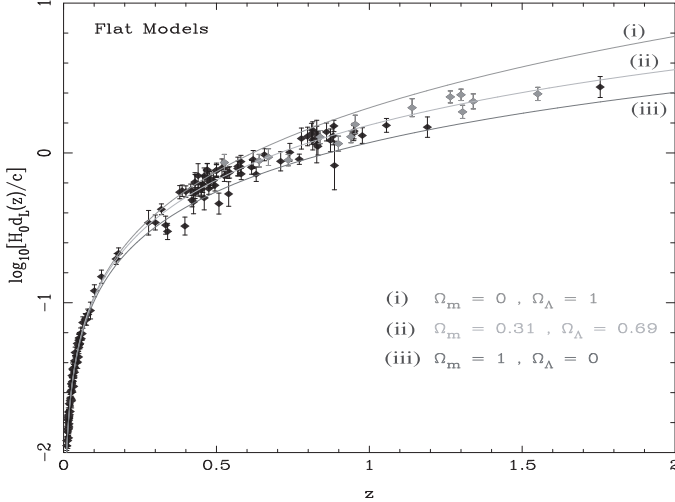


Fig. 5.2. The luminosity distance $d_L(z)$ versus the redshift z derived by SN Ia measurements. The black points with error bars correspond to “Gold” data sets [10]. Three theoretical curves represent those in the flat Λ CDM model with (i) $\Omega_m^{(0)} = 0$, $\Omega_{\text{DE}}^{(0)} = 1$, (ii) $\Omega_m^{(0)} = 0.31$, $\Omega_{\text{DE}}^{(0)} = 0.69$, and the Einstein de Sitter model (iii) $\Omega_m^{(0)} = 1$, $\Omega_{\text{DE}}^{(0)} = 0$. Reproduced from Ref. [11].

Universe. In Fig. 5.2, we also show “Gold” data sets [10] derived from SN Ia measurements. Clearly, the Universe with the cosmological constant is favored over the Einstein de Sitter model (case (iii) in Fig. 5.2).

In 1998, Perlmutter *et al.* [9] carried out the likelihood analysis by using 42 SN Ia data sets between $0.18 < z < 0.83$ together with 18 data sets perviously derived in low-redshift regimes ($z \ll 1$). For N data sets ($i = 1, 2, \dots, N$), the difference between the i th apparent magnitude $m(z_i)$ and absolute magnitude M is given by

$$\mu(z_i) \equiv m(z_i) - M = 5 \log_{10} \left(\frac{d_L(z_i)}{10 \text{ pc}} \right). \quad (5.18)$$

Denoting theoretical and observed values of $\mu(z_i)$ as $\mu_{\text{th}}(z_i)$ and $\mu_{\text{obs}}(z_i)$, respectively, the χ^2 associated with SN Ia observations is defined by

$$\chi_{\text{SNIa}}^2 = \sum_{i=1}^N \frac{[\mu_{\text{obs}}(z_i) - \mu_{\text{th}}(z_i)]^2}{\sigma_i^2}, \quad (5.19)$$

where σ_i represents errors due to flux uncertainties, intrinsic dispersion of SN Ia absolute magnitude, and peculiar velocity dispersion. The best fit corresponds to the case in which χ_{SNIa}^2 is minimized.

Assuming the flat Universe with the cosmological constant, Perlmutter *et al.* [9] derived the bound on the density parameter of non-relativistic matter as

$$\Omega_m^{(0)} = 0.28_{-0.08}^{+0.09} \quad (68\% \text{ CL}), \quad (5.20)$$

where the error represents a systematic one. The rest of the energy budget of the Universe (about 70%) constitutes dark energy responsible for the cosmic acceleration. Perlmutter *et al.* showed that the cosmological constant exists at more than 99% CL even by taking into account statistical errors. In 1998, Riess *et al.* [8] also reached the same conclusion from independent measurements of SN Ia in the redshift regime $z > 0.3$. After 1998, the fact that dark energy constitutes about 70% of today’s energy density of the Universe has been confirmed by other independent observations such as CMB and BAO.

The above results correspond to the flat Λ CDM model, i.e., $\Omega_{\mathcal{K}}^{(0)} = 0$ and $w_{\text{DE}} = -1$. The analysis can be extended to a more general situation in which the spatial curvature is present and w_{DE} is different from -1 . If w_{DE} is constant with $\Omega_{\mathcal{K}}^{(0)} \neq 0$, the normalized Hubble parameter becomes

$$E(z) = \left[\Omega_m^{(0)}(1+z)^3 + \Omega_{\text{DE}}^{(0)}(1+z)^{3(1+w_{\text{DE}})} + \Omega_{\mathcal{K}}^{(0)}(1+z)^2 \right]^{1/2}, \quad (5.21)$$

where we have set $\Omega_r^{(0)} = 0$ in Eq. (4.78). Substituting Eq. (5.21) into Eq. (5.13) and expanding the luminosity distance around $z = 0$, it follows that

$$d_L(z) = \frac{1}{H_0} \left[z + \frac{1}{4} \left(1 + \Omega_{\mathcal{K}}^{(0)} - 3w_{\text{DE}}\Omega_{\text{DE}}^{(0)} \right) z^2 + \mathcal{O}(z^3) \right]. \quad (5.22)$$

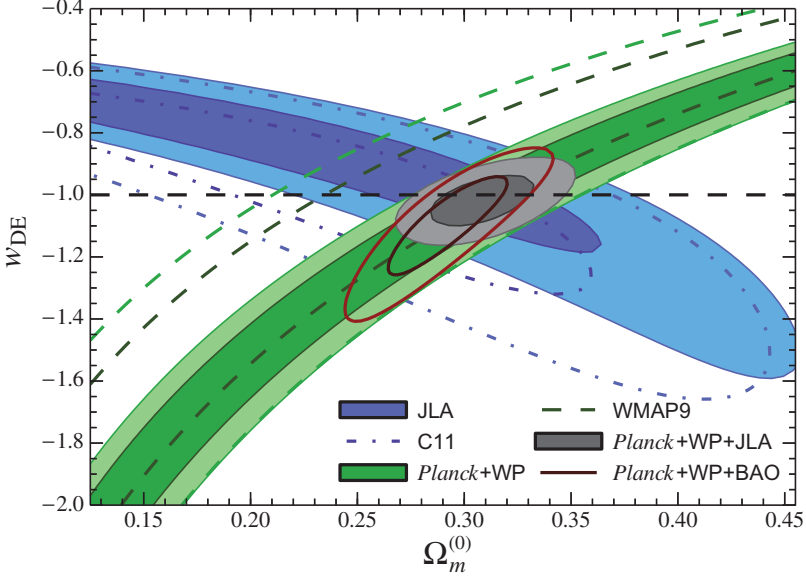


Fig. 5.3. Observational constraints on the constant dark energy equation of state w_{DE} in the flat Universe. The two curves in two filled contours represent 68% (inside) and 95% (outside) confidence level limits. The black dashed line corresponds to the Λ CDM model ($w_{\text{DE}} = -1$). “JLA” means the “joint light-curve analysis” provided by SNLS-SDSS supernovae surveys [12], whereas “C11” represents the SN Ia compilation of Conley *et al.* [13]. “Planck+WP” and “BAO” correspond to constraints derived from the CMB data of Planck/WMAP polarization [14] and the BAO data [15–17], respectively. The curves denoted as WMAP9 are bounds constrained from the WMAP 9-year data [18]. Reproduced from Ref. [12].

Since $\Omega_{\mathcal{K}}^{(0)} > 0$ in the open Universe, the luminosity distance is larger than that in the flat Universe. However, the present spatial curvature is as small as Eq. (4.81), so the open Universe without the cosmological constant cannot be consistent with the SN Ia data shown in Fig. 5.2.

Let us consider the flat Universe ($\Omega_{\mathcal{K}}^{(0)} = 0$) with the constant w_{DE} . From Eq. (5.22), it follows that the luminosity distance $d_L(z)$ gets larger for smaller w_{DE} with $\Omega_{\text{DE}}^{(0)} > 0$. In Fig. 5.3, we plot 68% and 95% observational contours in the $(w_{\text{DE}}, \Omega_m^{(0)})$ plane constrained by the joint light-curve analysis (JLA) of SNLS-SDSS supernovae surveys [12]. From the SN Ia data the dark energy equation of state is constrained to be $-1.6 < w_{\text{DE}} < -0.6$ at 95% confidence level. The constraints on w_{DE} and $\Omega_m^{(0)}$ are not very tight from the SN Ia data alone, but inclusion of other data such as CMB and BAO tightens the bounds on w_{DE} and $\Omega_m^{(0)}$. In Sec. 8 we will study how the property of dark energy can be constrained from observational data associated with the growth of inhomogeneities. The joint analysis based on the JLA+CMB+BAO data provide the bounds $w_{\text{DE}} = -1.027 \pm 0.055$ and $\Omega_m^{(0)} = 0.305 \pm 0.010$ (68% CL) [12].

5.3.3. Time-varying equation of state

So far we have studied the constant w_{DE} model, but most of theoretical dark energy models give rise to time-varying equations of state. The evolution of w_{DE} generally depends on models and initial conditions. Instead of considering specific models with concrete Lagrangians, several phenomenological parametrizations of w_{DE} were proposed to place constraints on the property of dark energy [19–28]. One example is given by the CPL parametrization [20, 21]

$$w_{\text{DE}}(a) = w_0 + w_a(1 - a), \quad (5.23)$$

where w_0, w_a are constants, and a is the scale factor with its present value $a_0 = 1$. For the parametrization (5.23) the present value of w_{DE} is w_0 , whereas $w_{\text{DE}} \rightarrow w_0 + w_a$ in the asymptotic past ($a \rightarrow 0$). Compared to the constant w_{DE} model, one more free parameter w_a is present, so there exists an additional degree of freedom for adjusting model parameters with observational data.

In Fig. 5.4, we show observational constraints on the model parameters (w_0, w_a) derived by the compilation of JLA SN Ia data [12] combined with CMB [14] and BAO [15–17] data. The JLA data alone put weak bounds on w_0 and w_a , but inclusion of the CMB and BAO data provide tighter constraints. The joint data analysis of JLA+CMB+BAO put the bounds $w_0 = -0.957 \pm 0.124$ and $w_a = -0.336 \pm 0.552$ (68% CL). Compared to the constant w_{DE} model, allowing the variation of w_{DE} leads to a wider parameter space consistent with observations. In Fig. 5.4, the cosmological constant ($w_0 = -1, w_a = 0$) is within the 68% CL contour constrained from the JLA+CMB+BAO data.

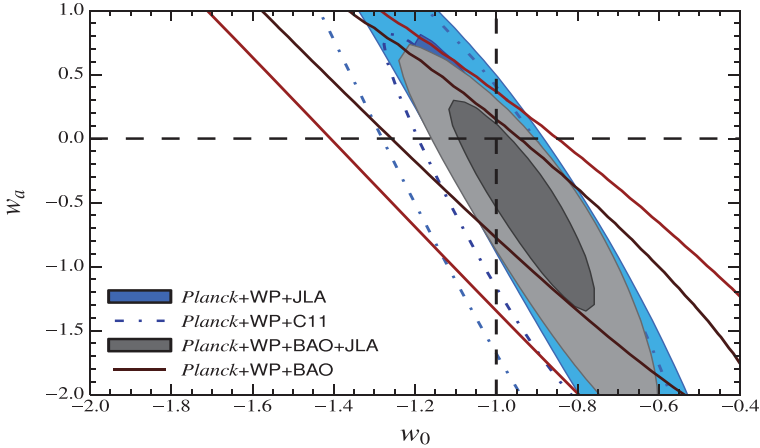


Fig. 5.4. Observational constraints on the model parameters (w_0, w_a) for the parametrization (5.23) in the flat Universe. The contours in the figure represent the 68% and 95% CL limits. The meanings of JLA, Planck, WP, BAO, C11 are the same as those given in the caption of Fig. 5.3. Reproduced from Ref. [12].

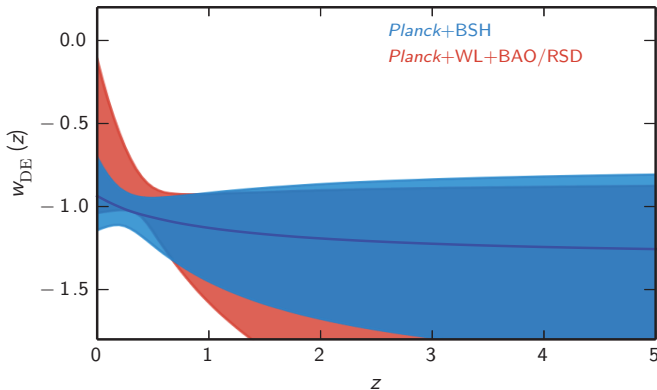


Fig. 5.5. Reconstructed dark energy equation of state $w_{\text{DE}}(z)$ constrained from different combinations of data sets derived by using the CPL parametrization (5.23) [29]. The labels BSH, WL, and RSD inside the figure indicate constraints derived from the data of BAO + SN Ia + H_0 , weak lensing, and red-shift space distortions, respectively. The best fit is shown as a solid line. Reproduced from Ref. [29].

In Fig. 5.5, the dark energy equation of state reconstructed from different combinations of data sets is shown as a function of z by using the parametrization (5.23) [29]. This shows that the models in which w_{DE} is larger than -0.8 at redshifts $z \gtrsim 0.5$ are disfavored from the data. On the other hand, the allowed parameter space in the region $w_{\text{DE}} < -1$ is wider than that for $w_{\text{DE}} > -1$. For dark energy models in the framework of GR, it is difficult to realize $w_{\text{DE}} < -1$ without having theoretical problems like ghosts. However, the realization of w_{DE} smaller than -1 is possible in modified gravity theories (as we will discuss in Chap. 11).

The two-parameter parametrization (5.23) was proposed for the purpose of placing constraints on dark energy in a model-independent way, but the cost of compression is that there exists a wide range of theoretical dark energy models whose variations of w_{DE} cannot be accommodated by (5.23). For example, the parametrization (5.23) does not allow models with fast transitions of w_{DE} . It is possible to encompass such models with the parametrization [26]

$$w_{\text{DE}}(a) = w_f + \frac{w_p - w_f}{1 + (a/a_t)^{1/\tau}}, \quad (5.24)$$

where $\tau (> 0)$ is the transition width, a_t characterizes the scale factor at transition, and w_p and w_f are asymptotic values of w_{DE} in the past and future, respectively (see also Refs. [23, 24] for related parametrizations). The parametrization (5.24) can approximately reproduce the evolution of w_{DE} for scaling quintessence models discussed later in Sec. 10.1.3.

There are also dark energy models in which w_{DE} has an extremum (like quintessence models in Ref. [30]). One example with an extremum at low redshifts

is given by the parametrization with four parameters w_p, w_0, a_t, τ [31]:

$$w_{\text{DE}}(a) = w_p + (w_0 - w_p) \frac{a^{1/\tau} [1 - (a/a_t)^{1/\tau}]}{1 - a_t^{-1/\tau}}. \quad (5.25)$$

In this case, w_{DE} has an extremum at $a = a_t/2^\tau$.

For the parametrizations (5.24) and (5.25), the joint likelihood analysis with SN Ia, CMB, and BAO data was carried out in Ref. [31]. It was shown that the total χ^2 can be smaller than that of the Λ CDM model. We need to caution however that these parametrizations have more free parameters than those in the Λ CDM model. To compare models with different number of free parameters, the Akaike Information Criterion (AIC) [32, 33]

$$\text{AIC} = \chi_{\text{min}}^2 + 2N_f \quad (5.26)$$

is often used. Here, χ_{min}^2 is the minimum value of χ^2 , and N_f is the number of free parameters for each model. The model with smaller AIC is more favored. If the difference of AIC between two models is in the range $0 < \Delta(\text{AIC}) < 2$, the models are considered to be equivalent. If $\Delta(\text{AIC}) > 2$, one model is favored over another. According to the AIC criterion, the four-parameter parametrizations (5.24) and (5.25) are not favored over the Λ CDM model in current observations [31, 34].

For given theoretical models with concrete Lagrangians, it is possible to derive analytic or numerical solutions to $w_{\text{DE}}(z)$ without resorting to phenomenological parametrizations explained above (as we will see in Chap. 10). In such cases, we can place observational constraints on each theoretical model and compare it with Λ CDM or other models in terms of the χ^2 statistics and the AIC.

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Chapter 6

Cosmological Perturbation Theory

To study the growth of structures in the Universe from a primordial era to today, we need to solve perturbed Einstein equations on the FLRW background in the presence of a fluid or a scalar field. We derive the equations of motion of linear cosmological perturbations by using a gauge-invariant formulation of perturbed quantities. In this and the rest of the chapters, we use the natural unit

$$c = \hbar = k_B = 1, \quad (6.1)$$

unless otherwise stated.

6.1. Perturbed line element on the FLRW background

Let us consider a perturbation $\delta g_{\mu\nu}$ of metric on the FLRW background. The background metric is given by $^{(b)}g_{\mu\nu}$ with the line element (4.1). Then, the metric can be written in the form

$$g_{\mu\nu} = ^{(b)}g_{\mu\nu} + \delta g_{\mu\nu}, \quad ^{(b)}g_{\mu\nu} = a^2(\eta) \begin{pmatrix} -1 & 0 \\ 0 & \gamma_{ii} \end{pmatrix}, \quad (6.2)$$

where γ_{ii} (with $i = 1, 2, 3$) are diagonal components of the three-dimensional spatial metric γ_{ij} ; see Eq. (4.2). Defining the conformal time η as

$$\eta \equiv \int a^{-1} dt, \quad (6.3)$$

the background line-element (4.1) can be expressed as

$$^{(b)}ds^2 = a^2(\eta)(-d\eta^2 + \gamma_{ij}dx^i dx^j). \quad (6.4)$$

As we will see below, the metric perturbation $\delta g_{\mu\nu}$ can be decomposed into three parts: (i) scalar, (ii) vector, and (iii) tensor. There are ten independent components of $\delta g_{\mu\nu}$ due to its symmetric property ($\delta g_{\mu\nu} = \delta g_{\nu\mu}$).

We begin with scalar perturbations. The time-time component δg_{00} has the contribution of a scalar quantity A , so it can be written in the form $\delta g_{00}^{(S)} = -2a^2(\eta)A$. The perturbation A depends on both time η and spatial position x^i . For the time-spatial components δg_{0i} and δg_{i0} , there is a contribution from a scalar perturbation B , such that $\delta g_{0i}^{(S)} = \delta g_{i0}^{(S)} = a^2(\eta)B_{|i}$. Here, $B_{|i}$ is the covariant derivative with respect to the three-dimensional spatial metric γ_{ij} . The spatial-spatial metric perturbation δg_{ij} has a contribution from two scalar quantities ψ and E , such that $\delta g_{ij}^{(S)} = 2a^2(\eta)(\psi\gamma_{ij} + E_{|ij})$. In summary, the perturbed metric associated with scalar perturbations is given by

$$\begin{aligned}\delta g_{00}^{(S)} &= -2a^2A, \\ \delta g_{0i}^{(S)} &= \delta g_{i0}^{(S)} = a^2B_{|i}, \\ \delta g_{ij}^{(S)} &= 2a^2(\psi\gamma_{ij} + E_{|ij}),\end{aligned}\tag{6.5}$$

with the four perturbations A , B , ψ , and E .

Let us next proceed to vector perturbations. The Helmholtz theorem states that an arbitrary three-dimensional spatial vector field V_i can be expressed as

$$V_i = S_i + B_{|i},\tag{6.6}$$

where S_i is a divergence-free vector obeying $S_i{}^{;i} = 0$ and $B_{|i}$ is a rotational-free vector satisfying $B_{|[ij]} \equiv (B_{|ij} - B_{|ji})/2 = 0$. Then, the perturbed metric δg_{0i} is composed of the intrinsic vector part $\delta g_{0i}^{(V)} = -a^2(\eta)S_i$ and the covariant derivative of intrinsic scalar part B . The metric δg_{ij} has the covariant derivative of a divergence-free vector F_i satisfying $F_i{}^{;i} = 0$. On using the symmetric property of metric, the contribution to δg_{ij} originating from the intrinsic vector mode can be written as $\delta g_{ij}^{(V)} = a^2(\eta)(F_{i|j} + F_{j|i})$. In summary, the perturbed metric related to the intrinsic vector mode is

$$\delta g_{0i}^{(V)} = \delta g_{i0}^{(V)} = -a^2S_i, \quad \delta g_{ij}^{(V)} = a^2(F_{i|j} + F_{j|i}),\tag{6.7}$$

where S_i and F_i obey the conditions:

$$S_i{}^{;i} = 0, \quad F_i{}^{;i} = 0.\tag{6.8}$$

Due to these two restrictions, there are $6-2=4$ components of vector perturbations S_i and F_i .

Finally, the contribution from tensor perturbations to the metric δg_{ij} is expressed in the form

$$\delta g_{ij}^{(T)} = a^2h_{ij}.\tag{6.9}$$

As in the case of vector perturbations, there is a decomposition theorem for a two-rank symmetric tensor T_{ij} [1]:

$$T_{ij} = T_{*ij} + \frac{1}{2}(T_{*i|j} + T_{*j|i}) + \left(S_{|ij} - \frac{1}{3}\gamma_{ij}\nabla^2 S\right) + \frac{1}{3}T\gamma_{ij}. \quad (6.10)$$

Here, T_{*ij} corresponds to the intrinsic tensor part obeying the two conditions $T_{*ij}{}^{||j} = 0$ and $T_{*i}{}^i = 0$. The second term on the right hand side of Eq. (6.10) is the contribution from the vector field T_{*i} . The last two terms correspond to contributions from the scalar quantity $S = (3/2)\Delta^{-1}(\Delta + 3\mathcal{K})^{-1}(T^{ij}{}_{|ij} - \Delta T/3)$ (where $\Delta \equiv \gamma^{ij}\nabla_i\nabla_j$) and the trace $T \equiv T^i{}_i$, respectively. From the theorem (6.10) the intrinsic tensor perturbation h_{ij} can be extracted according to

$$(i) \ h_{ij}{}^{||j} = 0 \quad (\text{divergenceless}), \quad (6.11)$$

$$(ii) \ h_i{}^i = 0 \quad (\text{traceless}). \quad (6.12)$$

These conditions give rise to three and one constraints, respectively. Hence there are $6 - 4 = 2$ components associated with tensor perturbations.

In summary, we have four scalar, four vector, and two tensor components, so there are ten components in total (which are the same as independent components of $\delta g_{\mu\nu}$). From Eqs. (6.5), (6.7), (6.9), the perturbed line element on the FLRW background is given by

$$ds^2 = a^2(\eta) \left\{ -(1 + 2A)d\eta^2 + 2(B_{|i} - S_i)d\eta dx^i + [(1 + 2\psi)\gamma_{ij} + 2E_{|ij} + 2F_{i|j} + h_{ij}]dx^i dx^j \right\}, \quad (6.13)$$

where all the perturbed quantities depend on η and x^i .

6.2. Gauge transformations

In GR, there exists a gauge degree of freedom associated with a general covariance of the theory. In linear perturbation theory, the gauge degree of freedom can be understood as the degree of freedom of an infinitesimal coordinate transformation. In this section, we study how perturbed quantities are transformed under such a gauge transformation.

We deal with spacetime as a manifold in which a local coordinate can be chosen at any point. Let us consider the following two manifolds [2]:

- (i) A manifold $\mathcal{M}$ containing perturbations on the FLRW background,
- (ii) A manifold $\mathcal{N}$ corresponding to the FLRW background.

We choose the coordinates x^μ and ${}^{(b)}x^\mu$ on the manifolds $\mathcal{M}$ and $\mathcal{N}$, respectively, and then consider the diffeomorphism $\mathcal{D} : {}^{(b)}x^\mu \rightarrow x^\mu$ between these two coordinates. A point P on $\mathcal{M}$ is transformed to the point $\mathcal{D}^{-1}(P)$ under the inverse

mapping $\mathcal{D}^{-1}$. A perturbation δT at the point P (δT can be scalar, vector, and tensor perturbations) is defined as

$$\delta T(x^\mu(P)) = T(x^\mu(P)) - {}^{(b)}T(\mathcal{D}^{-1}(P)), \quad (6.14)$$

where, for simplicity, we have expressed ${}^{(b)}T({}^{(b)}x^\mu(\mathcal{D}^{-1}(P)))$, as ${}^{(b)}T(\mathcal{D}^{-1}(P))$.

If we consider another diffeomorphism $\tilde{\mathcal{D}}: \mathcal{N} \rightarrow \mathcal{M}$, this leads to the transformation to another coordinate $\tilde{x}^\mu$ on $\mathcal{M}$, as $\tilde{\mathcal{D}}: {}^{(b)}x^\mu \rightarrow \tilde{x}^\mu$. In the coordinate $\tilde{x}^\mu$ we define the value of T at the point P , as $\tilde{T}(\tilde{x}^\mu(P))$. Since the background value of T corresponding to the point P is given by ${}^{(b)}T(\tilde{\mathcal{D}}^{-1}(P))$, the perturbation ${}^{(b)}T(\tilde{\mathcal{D}}^{-1}(P))$ in the new coordinate becomes

$$\widetilde{\delta T}(\tilde{x}^\mu(P)) = \tilde{T}(\tilde{x}^\mu(P)) - {}^{(b)}T(\tilde{\mathcal{D}}^{-1}(P)). \quad (6.15)$$

Let us consider the coordinate transformation

$$\tilde{x}^\mu = x^\mu + \xi^\mu. \quad (6.16)$$

If T is a scalar quantity f , then there is the relation $\tilde{f}(\tilde{x}^\mu) = f(x^\mu)$. Hence the perturbation (6.15) at the point P is

$$\begin{aligned} \widetilde{\delta f}(\tilde{x}^\mu) &= f(x^\mu) - {}^{(b)}f(\tilde{\mathcal{D}}^{-1}(P)) \\ &= f(\tilde{x}^\mu) - \xi^\mu \frac{\partial f}{\partial \xi^\mu}(\tilde{x}^\mu) - {}^{(b)}f(\tilde{\mathcal{D}}^{-1}(P)) \\ &= \delta f(\tilde{x}^\mu) - \xi^\mu \frac{\partial f}{\partial \tilde{x}^\mu}(\tilde{x}^\mu), \end{aligned} \quad (6.17)$$

where, in the second equality, we carried out the first-order expansion of ξ^μ . Since we are discussing a time-dependent background quantity ${}^{(b)}f = {}^{(b)}f(x^0)$, we obtain

$$\widetilde{\delta f} = \delta f - \xi^0 f', \quad (6.18)$$

where a prime represents a derivative with respect to $\tilde{x}^0 = \tilde{\eta}$.

Using the Helmholtz theorem for the vector $\tilde{x}^i$, the temporal and spatial parts of the infinitesimal coordinate transformation (6.16) can be expressed, respectively, as

$$\tilde{\eta} = \eta + \xi^0, \quad (6.19)$$

$$\tilde{x}^i = x^i + \xi^i + \zeta^i, \quad (6.20)$$

where $\xi^0 = \xi^0(\eta, x^i)$ and $\xi = \xi(\eta, x^i)$ are scalar functions, and $\zeta^i = \zeta^i(\eta, x^i)$ is a divergence-free vector satisfying $\zeta^i|_i = 0$. Since $\xi^0(\eta, x^i) = \xi^0(\tilde{\eta}, \tilde{x}^i)$, $\xi(\eta, x^i) = \xi(\tilde{\eta}, \tilde{x}^i)$, and $\zeta^i(\eta, x^i) = \zeta^i(\tilde{\eta}, \tilde{x}^i)$ at linear order of the infinitesimal transformation, we have

$$d\xi^0 = \xi^{0'} d\tilde{\eta} + \xi^0|_i d\tilde{x}^i, \quad (6.21)$$

$$d\xi = \xi' d\tilde{\eta} + \xi_{|j} d\tilde{x}^j, \quad (6.22)$$

$$d\zeta^i = \zeta^{i'} d\tilde{\eta} + \zeta^i_{|j} d\tilde{x}^j. \quad (6.23)$$

Then, from Eqs. (6.19) and (6.20), it follows that

$$d\eta = d\tilde{\eta} - \xi^{0'} d\tilde{\eta} - \xi^0_{|i} d\tilde{x}^i, \quad (6.24)$$

$$dx^i = d\tilde{x}^i - (\xi^{i'}_{|j} + \zeta^{i'}_{|j}) d\tilde{\eta} - (\xi^i_{|j} + \zeta^i_{|j}) d\tilde{x}^j. \quad (6.25)$$

For the scale factor $a(\eta)$, there is the relation

$$a(\eta) = a(\tilde{\eta} - \xi^0) = a(\tilde{\eta}) - \xi^0 a'(\tilde{\eta}). \quad (6.26)$$

The line element ds^2 is a scalar quantity invariant under the coordinate transformation, such that $d\tilde{s}^2 = ds^2$. Substituting Eqs. (6.24)–(6.26) into Eq. (6.13), the line element in the new coordinate $\tilde{x}^\mu$ is given by [2, 3]

$$\begin{aligned} ds^2 &= a^2(\tilde{\eta}) \{ - [1 + 2(A - \mathcal{H}\xi^0 - \xi^{0'})] d\tilde{\eta}^2 + 2(B + \xi^0 - \xi')_{|i} d\tilde{\eta} d\tilde{x}^i \\ &\quad - 2(S_i + \zeta'_i) d\tilde{\eta} d\tilde{x}^i + [(1 + 2(\psi - \mathcal{H}\xi^0))\gamma_{ij} + 2(E - \xi)_{|ij} \\ &\quad + 2(F_{i|j} - \zeta_{i|j}) + h_{ij}] d\tilde{x}^i d\tilde{x}^j \} \\ &\equiv a^2(\tilde{\eta}) \left\{ - (1 + 2\tilde{A}) d\tilde{\eta}^2 + 2(\tilde{B}_{|i} - \tilde{S}_i) d\tilde{\eta} d\tilde{x}^i \right. \\ &\quad \left. + [(1 + 2\tilde{\psi})\gamma_{ij} + 2\tilde{E}_{|ij} + 2\tilde{F}_{i|j} + \tilde{h}_{ij}] d\tilde{x}^i d\tilde{x}^j \right\}, \end{aligned} \quad (6.27)$$

where

$$\mathcal{H} = a'/a = aH = \dot{a}. \quad (6.28)$$

From Eq. (6.27), the scalar quantities A , B , ψ , E are subject to the following transformations:

$$\tilde{A} = A - \mathcal{H}\xi^0 - \xi^{0'}, \quad (6.29)$$

$$\tilde{B} = B + \xi^0 - \xi', \quad (6.30)$$

$$\tilde{\psi} = \psi - \mathcal{H}\xi^0, \quad (6.31)$$

$$\tilde{E} = E - \xi. \quad (6.32)$$

The vector perturbations F_i and S_i transform as

$$\tilde{F}_i = F_i - \zeta_i, \quad (6.33)$$

$$\tilde{S}_i = S_i + \zeta'_i. \quad (6.34)$$

The tensor perturbation is invariant under the gauge transformation

$$\tilde{h}_{ij} = h_{ij}. \quad (6.35)$$

6.3. Matter perturbations

In this section we study perturbations of the energy–momentum tensor $T^\mu{}_\nu$ appearing on the right hand side of Einstein equations (3.85). We also discuss how the matter perturbation $\delta T^\mu{}_\nu$ is affected by the gauge transformation (6.16). In the following, we will deal with the two cases: (i) a perfect fluid, and (ii) a scalar field, separately.

6.3.1. Perfect fluid

The energy–momentum tensor of a general fluid with energy density ρ and pressure P can be written as

$$T^\mu{}_\nu = (\rho + P)u^\mu u_\nu + P\delta^\mu_\nu + \pi^\mu{}_\nu. \quad (6.36)$$

The quantity $\pi^\mu{}_\nu$ is called an anisotropic stress tensor, which is related to the anisotropy in spatial dimensions. As given by Eq. (3.76), the perfect fluid does not have the anisotropic stress.

The four velocity of the fluid is defined by $u^\mu = dx^\mu/d\tau$, where τ is a proper time related to the infinitesimal line element ds according to $ds^2 = g_{\mu\nu}dx^\mu dx^\nu = -d\tau^2$ (such that the fluid is at rest ($dx^i = 0$) for the observer with a proper time clock). Then, the four velocity satisfies the relation $g_{\mu\nu}u^\mu u^\nu = -1$.

For the line element (6.13), the relation between τ and the conformal time η is given by $d\tau = a(1 + A)d\eta$. Then, the temporal component of u^μ is given by $u^0 = d\eta/d\tau = a^{-1}(1 + A)^{-1} \simeq a^{-1}(1 - A)$, where we employed the linear approximation in the second approximate equality. The spatial component of u^μ yields $u^i = dx^i/d\tau \simeq a^{-1}dx^i/d\eta$. From the Helmholtz theorem (6.6), the vector field $dx^i/d\eta$ can be expressed as the sum of scalar contribution $v_{|i}$ and intrinsic vector contribution v^i . The scalar v is a rotational-free velocity potential, whereas the vector v^i is a divergence-free vector satisfying $v^i{}_{|i} = 0$. In summary, the four-velocity can be written in the form

$$u^\mu = a^{-1}(1 - A, v_{|i} + v^i). \quad (6.37)$$

For the line-element (6.13), the covariant four-velocity reads

$$u_\nu = a(-1 - A, v_{|i} + B_{|i} + v_i - S_i). \quad (6.38)$$

On the FLRW background, we have $u^\mu = (a^{-1}, 0, 0, 0)$ and $u_\nu = (-a, 0, 0, 0)$, but in the presence of perturbations, the spatial components u^i (associated with peculiar velocities) do not vanish.

We write the energy density ρ and the pressure P in terms of background and perturbed parts, as $\rho = {}^{(b)}\rho + \delta\rho$ and $P = {}^{(b)}P + \delta P$. In the following, we omit the

index “(b)” for simplicity. The background parts obey the continuity equation

$$\rho' + 3\mathcal{H}(\rho + P) = 0, \quad (6.39)$$

where a prime represents a derivative with respect to η . Substituting Eqs. (6.37) and (6.38) into Eq. (6.36), we obtain each component of the energy–momentum tensor in the form

$$\begin{aligned} T^0_0 &= -\rho - \delta\rho, & T^0_i &= (\rho + P)(v_{|i} + B_{|i} + v_i - S_i), \\ T^i_0 &= -(\rho + P)(v_{|}^i + v^i), & T^i_j &= (P + \delta P)\delta_j^i + \pi^i_j. \end{aligned} \quad (6.40)$$

The anisotropic stress π^μ_ν has only the spatial component π^i_j . From the decomposition theorem analogous to Eq. (6.10), we can write π^i_j in the form

$$\pi^i_j = \left(\Pi_{|j}^i - \frac{1}{3}\nabla^2\Pi\delta_j^i \right) + \frac{1}{2}(\pi^i_{|j} + \pi_{j|}^i) + {}^{(T)}\pi^i_j, \quad (6.41)$$

where Π , $\pi^i_{|j}$, and ${}^{(T)}\pi^i_j$ correspond to the intrinsic scalar, vector, and tensor contributions, respectively. The last term on the right hand side of Eq. (6.10) appears as a pressure term in T^i_j of Eq. (6.40).

From the above discussion, the perturbations corresponding to scalar, vector, and tensor modes are given, respectively, by

(i) Scalar

$$\begin{aligned} {}^{(S)}\delta T^0_0 &= -\delta\rho, & {}^{(S)}\delta T^0_i &= (\rho + P)(v_{|i} + B_{|i}), \\ {}^{(S)}\delta T^i_0 &= -(\rho + P)v_{|}^i, & {}^{(S)}\delta T^i_j &= \delta P\delta_j^i + \Pi_{|j}^i - \frac{1}{3}\nabla^2\Pi\delta_j^i. \end{aligned} \quad (6.42)$$

(ii) Vector

$$\begin{aligned} {}^{(V)}\delta T^0_0 &= 0, & {}^{(V)}\delta T^0_i &= (\rho + P)(v_i - S_i), \\ {}^{(V)}\delta T^i_0 &= -(\rho + P)v^i, & {}^{(V)}\delta T^i_j &= \frac{1}{2}(\pi^i_{|j} + \pi_{j|}^i). \end{aligned} \quad (6.43)$$

(iii) Tensor

$${}^{(T)}\delta T^0_0 = 0, \quad {}^{(T)}\delta T^0_i = 0, \quad {}^{(T)}\delta T^i_0 = 0, \quad {}^{(T)}\delta T^i_j = {}^{(T)}\pi^i_j. \quad (6.44)$$

The scalar quantity f transforms as Eq. (6.18) under the infinitesimal shift (6.16), so the transformations associated with scalar perturbations $\delta\rho$ and δP are

$$\widetilde{\delta\rho} = \delta\rho - \rho'\xi^0, \quad \widetilde{\delta P} = \delta P - P'\xi^0. \quad (6.45)$$

As a next step, we consider the transformations of scalar part ${}^{(S)}\delta T^0_i$ and vector part ${}^{(V)}\delta T^0_i$ of the perturbation δT^0_i . Taking the η derivative of Eq. (6.20), we

obtain the relation $(\tilde{x}^i)' = (x^i)' + (\xi^i)' + (\zeta^i)'$. From this, the transformation of the scalar potential v is given by

$$\tilde{v} = v + \xi'. \quad (6.46)$$

The vector field v^i transforms as

$$\tilde{v}^i = v^i + (\zeta^i)'. \quad (6.47)$$

For later convenience we introduce the quantity

$$\delta q_i \equiv {}^{(S)}\delta T^0_i a, \quad (6.48)$$

which corresponds to momentum perturbations. For the perfect fluid, we have

$$\delta q = a(\rho + P)(v + B). \quad (6.49)$$

From Eqs. (6.30) and (6.46), the momentum perturbation δq is subject to the transformation

$$\tilde{\delta q} = \delta q + a(\rho + P)\xi^0. \quad (6.50)$$

Similarly, if we define

$${}^{(V)}\delta q_i \equiv {}^{(V)}\delta T^0_i a, \quad (6.51)$$

we have

$${}^{(V)}\delta q_i = a(\rho + P)(v_i - S_i). \quad (6.52)$$

From Eqs. (6.34) and (6.47), we find

$${}^{(V)}\tilde{\delta q}_i = {}^{(V)}\delta q_i. \quad (6.53)$$

Hence the perturbation ${}^{(V)}\delta q_i$ is invariant under the transformation (6.16). This property is called gauge-invariant.

6.3.2. Scalar field

Let us next proceed to the perturbation of a scalar field ϕ . We consider the case in which the field Lagrangian density $\mathcal{L}$ depends on ϕ and its kinetic energy $X = -g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi/2 \equiv -(\nabla\phi)^2/2$. The corresponding action is given by

$$S = \int d^4x \sqrt{-g} \mathcal{L}_\phi, \quad \mathcal{L}_\phi = P(\phi, X). \quad (6.54)$$

The Lagrangian density of a canonical scalar field with a potential $V(\phi)$ corresponds to $P = X - V(\phi)$. The model (6.54) can accommodate the case in which $\mathcal{L}_\phi$ contains a non-linear function in X . Such non-linear kinetic terms can give rise to the cosmic acceleration even without the field potential [4–6].

The energy-momentum tensor $T_{\mu\nu}$ follows from the Lagrangian density $\mathcal{L}_\phi$ according to the relation (4.92). For the Lagrangian density $\mathcal{L}_\phi = P(\phi, X)$, we have $T_{\mu\nu} = P_{,X} \nabla_\mu \phi \nabla_\nu \phi + g_{\mu\nu} P$, where $P_{,X} \equiv \partial P / \partial X$. Hence the mixed energy-momentum tensor yields

$$T^\lambda{}_\nu = P_{,X} \nabla^\lambda \phi \nabla_\nu \phi + \delta^\lambda_\nu P. \quad (6.55)$$

Decomposing the scalar field into the background and perturbed components as $\phi(\eta, x^i) = {}^{(b)}\phi(\eta) + \delta\phi(\eta, x^i)$, the background energy density is given by

$$\rho = -{}^{(b)}T^0{}_0 = a^{-2} P_{,X} \phi'^2 - P = 2X P_{,X} - P, \quad (6.56)$$

where we omitted the index “(b)” in the second equality and we used the relation $X = (1/2)a^{-2}\phi'^2$. The field pressure ${}^{(b)}T^i{}_i/3$ corresponds to the Lagrangian density P itself. The energy density ρ and the pressure P obey the continuity equation (6.39).

For the line-element (6.13), the perturbed components of the energy-momentum tensor (6.55) yield

$$\delta\rho \equiv -\delta T^0{}_0 = (P_{,X} + 2X P_{,XX}) \delta X - (P_{,\phi} - 2X P_{,X\phi}) \delta\phi, \quad (6.57)$$

$$\delta q_{|i} \equiv a \delta T^0{}_i = -a^{-1} P_{,X} \phi' \delta\phi_{|i}, \quad (6.58)$$

$$\delta P \delta^i{}_j \equiv \delta T^i{}_j = (P_{,X} \delta X + P_{,\phi} \delta\phi) \delta^i{}_j, \quad (6.59)$$

where $P_{,X\phi} \equiv \partial^2 P / (\partial\phi \partial X)$, and

$$\delta X = a^{-2} (\phi' \delta\phi' - A \phi'^2). \quad (6.60)$$

Since ϕ is a scalar quantity, it is transformed as

$$\widetilde{\delta\phi} = \delta\phi - \phi' \xi^0. \quad (6.61)$$

The perturbations $\delta\rho$ and δP are also subject to the transformation same as Eq. (6.45). From Eq. (6.58), the momentum perturbation δq is given by

$$\delta q = -a^{-1} P_{,X} \phi' \delta\phi. \quad (6.62)$$

From Eqs. (6.56) and (6.61), the perturbation δq obeys the transformation in the same way as Eq. (6.50).

6.4. Gauge-invariant quantities and gauge fixing

In Secs. 6.2 and 6.3, we studied how metric perturbations and matter perturbations are subject to change under the gauge transformation (6.16). In this section, we construct several gauge-invariant quantities unaffected by the gauge transformation and also discuss several different gauge choices.

6.4.1. Gauge-invariant quantities

Let us consider perturbed quantities invariant under the transformation (6.16). Two gauge-invariant quantities constructed from metric perturbations A , B , E , ψ are given by

$$\Psi \equiv A - \frac{1}{a} [a(E' - B)]', \quad (6.63)$$

$$\Phi \equiv \psi - \mathcal{H}(E' - B). \quad (6.64)$$

From Eqs. (6.29)–(6.32), it follows that $\tilde{\Psi} = \Psi$ and $\tilde{\Phi} = \Phi$. The quantities Ψ and Φ are called Bardeen gravitational potentials [7].

The following three quantities introduced in Refs. [8–11] are also gauge-invariant:

$$\mathcal{R} \equiv \psi + \frac{H}{\rho + P} \delta q, \quad (6.65)$$

$$\zeta \equiv \psi - \frac{\mathcal{H}}{\rho'} \delta \rho, \quad (6.66)$$

$$\delta \phi_\psi \equiv \delta \phi - \frac{\phi'}{\mathcal{H}} \psi. \quad (6.67)$$

For the scalar field ϕ , we can express $\mathcal{R}$ in the form

$$\mathcal{R} = \psi - \frac{\mathcal{H}}{\phi'} \delta \phi, \quad (6.68)$$

where we used Eqs. (6.56) and (6.62). From Eqs. (6.45), (6.50) and (6.39), the combination

$$\delta \rho_m \equiv \delta \rho - 3H \delta q \quad (6.69)$$

is also gauge-invariant. The perturbations $\mathcal{R}$ and ζ are related to each other, as

$$\mathcal{R} = \zeta + \frac{\mathcal{H}}{\rho'} \delta \rho_m. \quad (6.70)$$

The gauge-invariant perturbation $\delta \phi_\psi$ is related to $\mathcal{R}$, as $\delta \phi_\psi = -(\phi'/\mathcal{H})\mathcal{R}$.

For the vector perturbations S_i and F_i , we have $\tilde{S}_i + \tilde{F}_i' = S_i + F_i'$ from Eqs. (6.33) and (6.34), so the quantity

$$U_i \equiv S_i + F_i' \quad (6.71)$$

is gauge-invariant.

6.4.2. Gauge fixing

For the gauge transformation (6.16), the two scalar quantities ξ^0, ξ , and the vector ζ^i ($i = 1, 2, 3$) are not fixed yet. Since ζ^i is subject to the constraint $\zeta^i|_i = 0$, there are four gauge degrees of freedom in total. These four degrees of freedom are determined by choosing a gauge. After choosing $\tilde{F}_i = 0$ in Eq. (6.33), we can fix $\zeta_i = F_i$. The remaining gauge degrees of freedom to be fixed are two, i.e., ξ^0 and ξ . In the following, we consider several different gauge fixings for scalar perturbations.

(A) Newtonian gauge

The Newtonian gauge corresponds to $\tilde{B} = 0$ and $\tilde{E} = 0$. From Eqs. (6.30) and (6.32), ξ^0 and ξ are fixed as

$$\xi^0 = E' - B, \quad \xi = E. \quad (6.72)$$

Substituting these into Eqs. (6.29) and (6.31), we obtain $\tilde{A} = \Psi$ and $\tilde{\psi} = \Phi$, where Ψ and Φ are Bardeen potentials defined by Eqs. (6.63) and (6.64). Then, the line element in the Newtonian gauge becomes

$$ds^2 = a^2(\eta)[-(1 + 2\Psi)d\eta^2 + (1 + 2\Phi)\gamma_{ij}dx^i dx^j], \quad (6.73)$$

where we omitted the tilde in metric perturbations after the gauge transformation.

(B) Spatially flat gauge

Let us consider the spatially flat gauge in which perturbations in the spatial metric vanish, i.e., $\tilde{\psi} = 0$ and $\tilde{E} = 0$. Then, the gauge is fixed to be

$$\xi^0 = \frac{\psi}{\mathcal{H}}, \quad \xi = E. \quad (6.74)$$

Other metric perturbations are given by

$$\tilde{A} = A - \psi - \left(\frac{\psi}{\mathcal{H}}\right)', \quad \tilde{B} = B + \frac{\psi}{\mathcal{H}} - E'. \quad (6.75)$$

For this gauge choice, we have $\widetilde{\delta\phi}_\psi = \widetilde{\delta\phi}$, $\widetilde{\mathcal{R}} = -(\mathcal{H}/\phi')\widetilde{\delta\phi}_\psi$, and $\tilde{\zeta} = -(\mathcal{H}/\rho')\tilde{\delta\rho}$.

(C) Uniform-density gauge

The uniform-density gauge corresponds to the gauge choice $\tilde{\delta\rho} = 0$. From Eq. (6.45), we have

$$\xi^0 = \frac{\delta\rho}{\rho'}, \quad (6.76)$$

whereas ξ can be fixed by choosing $\tilde{B} = 0$ or $\tilde{E} = 0$. Under this gauge choice we have $\tilde{\zeta} = \tilde{\psi}$. The three-dimensional spatial curvature on constant-time hypersurfaces is given by

$${}^{(3)}\mathcal{R} = \frac{6}{a^2} (1 - 2\psi) \mathcal{K} - \frac{4}{a^2} \nabla^2 \psi, \quad (6.77)$$

where ∇^2 is the three-dimensional Laplacian. In the flat Universe ($\mathcal{K} = 0$) the metric perturbation ψ is directly related to ${}^{(3)}\mathcal{R}$, as ${}^{(3)}\mathcal{R} = -(4/a^2) \nabla^2 \psi$. Hence ζ is often called the curvature perturbation on constant-density hypersurfaces.

(D) Comoving gauge

For the perfect fluid, the coming gauge corresponds to choosing $\tilde{v} = 0$ and $\tilde{B} = 0$. From Eqs. (6.30) and (6.46), we have

$$\xi^{(0)} = -v - B, \quad \xi = - \int v d\eta + Y(x^i), \quad (6.78)$$

where $Y(x^i)$ is a scalar quantity that depends on the spatial coordinate x^i . The perturbation $\tilde{E}$ is affected by the uncertainty of $Y(x^i)$, while $\tilde{A}$, $\tilde{B}$, and $\tilde{\psi}$ are fixed. Meanwhile, the time derivative $\tilde{E}'$ does not have the uncertainty of $Y(x^i)$, so the quantities Ψ and Φ in Eqs. (6.63) and (6.64) are fixed. Moreover, for scalar quantities like $\delta\rho$, δP , $\delta\phi$, δq , v , the associated gauge transformation contains ξ^0 and ξ' instead of ξ itself. Hence the uncertainty of ξ originating from $Y(x^i)$ is not problematic. Since $\tilde{\delta}q = 0$ for the coming gauge, we have $\tilde{\mathcal{R}} = \tilde{\psi}$ from Eq. (6.68). Since ψ is related to the three-dimensional spatial curvature ${}^{(3)}\mathcal{R}$ as Eq. (6.77), we often call $\mathcal{R}$ the coming curvature perturbation.

For the scalar field ϕ the coming gauge corresponds to $\tilde{\delta}q = 0$, which translates to $\tilde{\delta}\phi = 0$ from Eq. (6.62). In this case, the coming gauge is often called the unitary gauge. From the transformation law (6.61), we have $\xi^0 = \delta\phi/\phi'$ and ξ can be also fixed by choosing $\tilde{E} = 0$ (in which case $\xi = E$).

(E) Synchronous gauge

The synchronous gauge, which was first introduced by Lifschitz, corresponds to $\tilde{A} = 0$ and $\tilde{B} = 0$. If $\xi^0 = \bar{\xi}^0$ is a solution to $0 = A - \mathcal{H}\xi^0 - \xi^{0'}$, there is another solution $\xi^0 = \bar{\xi}^0 + a^{-1}Z(x^i)$, where $Z(x^i)$ is a function that depends on x^i . Then, most of perturbed quantities are affected by the uncertainty of ξ^0 . Due to the historical reason, this gauge was often used to discuss the evolution of perturbations during radiation- or matter-dominated epochs, but we need to be careful for the above uncertainty of gauge fixing.

We can choose a most convenient gauge depending on problems at hand. The physics is not affected by the choice of gauges (apart from the case of choosing the synchronous gauge).

6.5. Perturbed Einstein equations

In theories within the framework of GR, we derive linear perturbation equations of motion on the FLRW background. We do not fix the gauge in this section, so the resulting equations of motion are valid for any gauge choice. The Einstein tensor $G^\mu{}_\nu$ and the energy–momentum tensor $T^\mu{}_\nu$ can be decomposed into the background and perturbed parts, as $G^\mu{}_\nu = {}^{(b)}G^\mu{}_\nu + \delta G^\mu{}_\nu$ and $T^\mu{}_\nu = {}^{(b)}T^\mu{}_\nu + \delta T^\mu{}_\nu$, respectively. The background equations ${}^{(b)}G^\mu{}_\nu = 8\pi G {}^{(b)}T^\mu{}_\nu$ give rise to Eqs. (4.15) and (4.16) with the continuity equation (6.39). The linearly perturbed Einstein equations without the cosmological constant are given by

$$\delta G^\mu{}_\nu = 8\pi G \delta T^\mu{}_\nu. \quad (6.79)$$

As for the perturbed energy–momentum tensors $\delta T^\mu{}_\nu$, we already derived them for the fluid and the scalar field in Sec. 6.3.

Let us obtain the perturbed Einstein tensor $\delta G^\mu{}_\nu$ for the line element (6.13). First, the perturbed Christoffel symbols are given by

$$\delta \Gamma^\mu_{\nu\lambda} = \frac{1}{2} \delta g^{\mu\alpha} (g_{\alpha\nu,\lambda} + g_{\alpha\lambda,\nu} - g_{\nu\lambda,\alpha}) + \frac{1}{2} g^{\mu\alpha} (\delta g_{\alpha\nu,\lambda} + \delta g_{\alpha\lambda,\nu} - \delta g_{\nu\lambda,\alpha}). \quad (6.80)$$

The next step is to compute the perturbations of Ricci tensor $R_{\mu\nu}$ and Ricci scalar R , according to the formulas:

$$\delta R_{\mu\nu} = \delta \Gamma^\alpha_{\mu\nu,\alpha} - \delta \Gamma^\alpha_{\mu\alpha,\nu} + \delta \Gamma^\alpha_{\mu\nu} \Gamma^\beta_{\alpha\beta} + \Gamma^\alpha_{\mu\nu} \delta \Gamma^\beta_{\alpha\beta} - \delta \Gamma^\alpha_{\mu\beta} \Gamma^\beta_{\alpha\nu} - \Gamma^\alpha_{\mu\beta} \delta \Gamma^\beta_{\alpha\nu}, \quad (6.81)$$

$$\delta R = \delta g^{\mu\nu} R_{\mu\nu} + g^{\mu\nu} \delta R_{\mu\nu}. \quad (6.82)$$

Finally, we can derive the perturbed Einstein tensor as

$$\delta G^\mu{}_\nu = R^\mu{}_\nu - \frac{1}{2} \delta^\mu_\nu \delta R. \quad (6.83)$$

Below, we present the perturbed Einstein tensors corresponding to scalar, vector, and tensor perturbations, respectively.¹

(i) Scalar perturbations

$${}^{(S)}\delta G^0{}_0 = 2a^{-2} [3\mathcal{H}(\mathcal{H}A - \psi') + \nabla^2 \{\psi - \mathcal{H}(E' - B)\} + 3\mathcal{K}\psi], \quad (6.84)$$

$${}^{(S)}\delta G^0{}_i = -2a^{-2} [\mathcal{H}A - \psi' + \mathcal{K}(E' - B)]_{|i}, \quad (6.85)$$

¹The computations of perturbed geometric quantities are straightforward but quite cumbersome. The calculations can be easily done by using computer softwares like **Maple** or **Mathematica**.

$${}^{(S)}\delta G^i_j = 2a^{-2} [(\mathcal{H}^2 + 2\mathcal{H}')A + \mathcal{H}A' - \psi'' - 2\mathcal{H}\psi' + \mathcal{K}\psi] \delta^i_j + a^{-2} (\nabla^2 D \delta^i_j - D|{}^i_j), \quad (6.86)$$

where

$$D \equiv A + \psi - 2\mathcal{H}(E' - B) - (E' - B)'. \quad (6.87)$$

Taking the trace of Eq. (6.86) leads to

$${}^{(S)}\delta G^i_i = 6a^{-2} [(\mathcal{H}^2 + 2\mathcal{H}')A + \mathcal{H}A' - \psi'' - 2\mathcal{H}\psi' + \mathcal{K}\psi] + 2a^{-2}\nabla^2 D. \quad (6.88)$$

(ii) Vector perturbations

$${}^{(V)}\delta G^0_0 = 0, \quad (6.89)$$

$${}^{(V)}\delta G^0_i = -\frac{2\mathcal{K} + \nabla^2}{2a^2}(S_i + F'_i), \quad (6.90)$$

$${}^{(V)}\delta G^i_j = \frac{1}{2}a^{-2} \left\{ \left(\frac{\partial}{\partial \eta} + 2\mathcal{H} \right) [S^i_{|j} + S_j|^i + (F^i_{|j} + F_j|^i)'] \right\}. \quad (6.91)$$

(iii) Tensor perturbations

$${}^{(T)}\delta G^0_0 = 0, \quad (6.92)$$

$${}^{(T)}\delta G^0_i = 0, \quad (6.93)$$

$${}^{(T)}\delta G^i_j = \frac{1}{2}a^{-2}[(h^i_j)'' + 2\mathcal{H}(h^i_j)' + (2\mathcal{K} - \nabla^2)h^i_j]. \quad (6.94)$$

In what follows, we consider the perturbed Einstein equations for the fluid and the scalar field, separately.

6.5.1. Fluid

On using the perturbed energy–momentum tensor derived in Sec. 6.3, we now derive the equations of motion for scalar, vector, and tensor perturbations for the fluid. On the FLRW background, we can express Eqs. (4.15) and (4.16) in the forms

$$3\mathcal{H}^2 = 8\pi G a^2 \rho - 3\mathcal{K}, \quad (6.95)$$

$$\mathcal{H}' - \mathcal{H}^2 = -4\pi G a^2 (\rho + P) + \mathcal{K}, \quad (6.96)$$

together with the continuity equation (6.39).

(i) Scalar perturbation equations

From the (00) and (0i) components of perturbed Einstein equations, it follows that

$$3\mathcal{H}(\psi' - \mathcal{H}A) - (\nabla^2 + 3\mathcal{K})\psi + \mathcal{H}\nabla^2\sigma = 4\pi G a^2 \delta\rho, \quad (6.97)$$

$$\psi' - \mathcal{H}A - \mathcal{K}\sigma = 4\pi G a \delta q, \quad (6.98)$$

where

$$\sigma \equiv E' - B, \quad (6.99)$$

and we used $\delta q = a(\rho + P)(v + B)$. For $i \neq j$, we have ${}^{(S)}\delta G^i_j = -a^{-2}D^i_j$ and ${}^{(S)}\delta T^i_j = \Pi^i_j$, so the perturbed Einstein equation ${}^{(S)}\delta G^i_j = 8\pi G {}^{(S)}\delta T^i_j$ gives $D = -8\pi G a^2 \Pi$, i.e.,

$$\sigma' + 2\mathcal{H}\sigma - A - \psi = 8\pi G a^2 \Pi. \quad (6.100)$$

Employing Eq. (6.88) and the relation ${}^{(S)}\delta T^i_i = 3\delta P$, we obtain

$$\psi'' + 2\mathcal{H}\psi' - \mathcal{K}\psi - \mathcal{H}A' - (\mathcal{H}^2 + 2\mathcal{H}')A = -4\pi G a^2 \left(\delta P + \frac{2}{3}\nabla^2 \Pi \right). \quad (6.101)$$

In terms of the gauge-invariant gravitational potentials Ψ, Φ defined by Eqs. (6.63)–(6.64), we can write Eq. (6.100) in the form

$$\Psi + \Phi = -8\pi G a^2 \Pi. \quad (6.102)$$

In the absence of the anisotropic stress ($\Pi = 0$), we have that $\Psi = -\Phi$.

From the continuity equations $T^\mu_{0;\mu} = 0$ and $T^\mu_{i;\mu} = 0$, it is also possible to derive the perturbation equations for $\delta\rho$ and δq . The first continuity equation corresponds to

$$T^\mu_{0;\mu} = \frac{\partial T^0_0}{\partial \eta} + \frac{\partial T^i_0}{\partial x^i} + \Gamma^i_{i0}T^0_0 - \Gamma^i_{i0}T^i_i = 0. \quad (6.103)$$

On using the background continuity equation (6.39), the perturbed part reads

$$\delta T^\mu_{0;\mu} = -\delta\rho' - 3\mathcal{H}(\delta\rho + \delta P) - (\rho + P) [3\psi' + \nabla^2(E' + v)], \quad (6.104)$$

so the first perturbed continuity equation $\delta T^\mu_{0;\mu} = 0$ leads to

$$\delta\rho' + 3\mathcal{H}(\delta\rho + \delta P) = -(\rho + P) [3\psi' + \nabla^2(E' + v)]. \quad (6.105)$$

Similarly we have

$$\delta T^\mu_{i;\mu} = a^{-1} \left[\delta q' + 3\mathcal{H}\delta q + a\delta P + \frac{2}{3}a(\nabla^2 + 3\mathcal{K})\Pi + (\rho + P)aA \right]_{|i}, \quad (6.106)$$

so the second perturbed continuity equation $\delta T^\mu_{i;\mu} = 0$ gives

$$\delta q' + 3\mathcal{H}\delta q = -a\delta P - \frac{2}{3}a(\nabla^2 + 3\mathcal{K})\Pi - (\rho + P)aA. \quad (6.107)$$

We can also derive Eqs. (6.105) and (6.107) by using Eqs. (6.97)–(6.101).

(ii) Vector perturbed equations

The (00) component of perturbed Einstein equations is related to scalar quantities, so there is no corresponding vector perturbation equation. From the (0*i*) and

(ij) components of perturbed Einstein equations, the vector perturbations F_i , S_i , and v_i obey

$$(\nabla^2 + 2\mathcal{K})(F'_i + S_i) = -16\pi G a^{(V)} \delta q_i, \quad (6.108)$$

$$\tau^i_{j'} + 3\mathcal{H}\tau^i_j = 4\pi G a(\pi^i_{|j} + \pi_{|j}^i), \quad (6.109)$$

where $^{(V)}\delta q_i = a(\rho + P)(v_i - S_i)$, and

$$\tau^i_j \equiv \frac{1}{2a} [S^i_{|j} + S_{|j}^i + (F^i_{|j} + F_{|j}^i)']. \quad (6.110)$$

From the continuity equation $T^\mu_{i;\mu} = 0$, we obtain

$$^{(V)}\delta q'_i + 3\mathcal{H}^{(V)}\delta q_i = -a(\nabla^2 + 2\mathcal{K})\pi_i, \quad (6.111)$$

whereas there is no equation following from $T^\mu_{0;\mu} = 0$.

(iii) Tensor perturbation equations

The perturbed Einstein equation $^{(T)}\delta G^i_j = 8\pi G^{(T)}\delta T^i_j$ of tensor perturbations corresponds to

$$(h^i_j)'' + 2\mathcal{H}(h^i_j)' + (2\mathcal{K} - \nabla^2)h^i_j = 16\pi G^{(T)}\pi^i_j a^2. \quad (6.112)$$

In the absence of the anisotropic stress ($^{(T)}\pi^i_j=0$), the perturbation h^i_j satisfies the simple second-order differential equation uncoupled to other perturbed quantities.

6.5.2. Scalar field

Let us consider a scalar field ϕ described by the k-essence Lagrangian density $P(\phi, X)$. The background equations of motion are the same as Eqs. (6.95) and (6.96) when replacing ρ with $2XP_{,X} - P$. The background continuity equation (6.39) can be written as

$$(P_{,X} + 2XP_{,XX})\phi'' + 2(P_{,X} - XP_{,XX})\mathcal{H}\phi' + a^2(2XP_{,X\phi} - P_{,\phi}) = 0. \quad (6.113)$$

The perturbed energy-momentum tensors are given by Eqs. (6.57)–(6.59). Comparing them with those of the fluid, the scalar field corresponds to $v_i = S_i = \pi_i = 0$ and $\pi^i_j = 0$.

(i) Scalar perturbation equations

For scalar perturbations, the (00) , $(0i)$, (ij) [$i \neq j$] components of the Einstein equations and the trace equation correspond to

$$\begin{aligned} & 3\mathcal{H}\psi' - [3\mathcal{H}^2 - 4\pi G\phi'^2(P_{,X} + 2XP_{,XX})]A - (\nabla^2 + 3\mathcal{K})\psi + \mathcal{H}\nabla^2\sigma \\ & = -4\pi G[a^2(P_{,\phi} - 2XP_{,X\phi})\delta\phi - (P_{,X} + 2XP_{,XX})\phi'\delta\phi'], \end{aligned} \quad (6.114)$$

$$\psi' - \mathcal{H}A - \mathcal{K}\sigma = -4\pi G P_{,X} \phi' \delta\phi, \quad (6.115)$$

$$\sigma' + 2\mathcal{H}\sigma - A - \psi = 0, \quad (6.116)$$

$$\begin{aligned} \psi'' + 2\mathcal{H}\psi' - \mathcal{K}\psi - \mathcal{H}A' - (2\mathcal{H}^2 + \mathcal{H}' + \mathcal{K})A \\ = -4\pi G (P_{,X} \phi' \delta\phi' + a^2 P_{,\phi} \delta\phi), \end{aligned} \quad (6.117)$$

where we used Eq. (6.96). The perturbations $\delta\rho$ and δP associated with the scalar field obey Eq. (6.105), i.e.,

$$\delta\rho' + 3\mathcal{H}(\delta\rho + \delta P) = -a^{-1}\nabla^2\delta q - (\rho + P)(3\psi' + \nabla^2\sigma). \quad (6.118)$$

This is not independent of Eqs. (6.114)–(6.117). The equation (6.107) of the momentum perturbation δq is automatically satisfied.

(ii) Vector perturbation equations

As we already pointed it out, the quantities v_i , S_i , π_i vanish for the scalar field. Hence the terms on the right hand side of Eqs. (6.108), (6.109) and (6.111) vanish, so that

$$(\nabla^2 + 2\mathcal{K})(F'_i + S_i) = 0, \quad (6.119)$$

$$\tau^{i,j'} + 3\mathcal{H}\tau^i_j = 0, \quad (6.120)$$

$${}^{(V)}\delta q'_i + 3\mathcal{H}{}^{(V)}\delta q_i = 0. \quad (6.121)$$

From Eq. (6.119), the perturbation $F'_i + S_i$ does not grow in time. From Eqs. (6.120) and (6.121), both τ^i_j and ${}^{(V)}\delta q_i$ decrease in proportion to a^{-3} . Thus, the vector perturbation associated with the scalar field does not have a growing mode.

(iii) Tensor perturbation equations

Since ${}^{(T)}\pi^i_j = 0$ for the scalar field, the tensor perturbation h^i_j obeys the second-order differential equation:

$$(h^i_j)'' + 2\mathcal{H}(h^i_j)' + (2\mathcal{K} - \nabla^2)h^i_j = 0. \quad (6.122)$$

In the large-scale limit we have $\nabla^2 h^i_j \rightarrow 0$, so Eq. (6.122) admits the solution with constant h^i_j . In fact, this is a growing-mode solution relevant to the generation of primordial tensor perturbations during inflation.

Since the momentum perturbation δq of the scalar field is given by Eq. (6.62), Eq. (6.115) is of the same form as Eq. (6.98). On using this latter equation for $\mathcal{K} = 0$, the coming curvature perturbation $\mathcal{R}$ defined by Eq. (6.65) can be expressed as

$$\mathcal{R} = \psi - \frac{2}{3(1+w)} \left(\mathcal{A} - \frac{\psi'}{\mathcal{H}} \right), \quad (6.123)$$

where we used Eq. (6.95) and the equation of state $w = P/\rho$. In terms of the Bardeen potentials Ψ and Φ , Eq. (6.123) can be written in the form

$$\mathcal{R} = \Phi - \frac{2}{3(1+w)} \left(\Psi - \frac{\Phi'}{\mathcal{H}} \right). \quad (6.124)$$

In the absence of the anisotropic stress Π , we have $\Psi = -\Phi$ from Eq. (6.102). If Φ is constant in Eq. (6.124), it follows that

$$\mathcal{R} = \frac{5+3w}{3(1+w)} \Phi, \quad (6.125)$$

which is often used to relate the curvature perturbation $\mathcal{R}$ generated during inflation with the gravitational potential Φ in the radiation- and matter-dominated epochs.

6.6. Entropy perturbations and the sound speed

For a perfect fluid with pressure P and density ρ , the sound speed c_a is adiabatic and its square is given by

$$c_a^2 = \frac{\dot{P}}{\dot{\rho}} = w - \frac{w'}{3\mathcal{H}(1+w)}, \quad (6.126)$$

where $w = P/\rho$. On the other hand, for an imperfect fluid like a scalar field, there is an entropy production due to dissipations. In this case, the sound speed squared is given by

$$c_s^2 = \frac{\delta P}{\delta \rho}, \quad (6.127)$$

which is different from Eq. (6.126). We define the entropy perturbation δs in terms of the difference between c_s^2 and c_a^2 multiplied by $\delta = \delta\rho/\rho$, as [1, 12]

$$\delta s = (c_s^2 - c_a^2) \delta = \frac{\dot{P}}{\rho} \left(\frac{\delta P}{\dot{P}} - \frac{\delta \rho}{\dot{\rho}} \right). \quad (6.128)$$

From Eq. (6.45), the entropy perturbation is gauge-invariant.

The quantity c_s^2 defined by Eq. (6.127) generally depends on the gauge choice. To remove such dependence, we introduce the following gauge-invariant quantity

$$\delta_m \equiv \frac{\delta \rho_m}{\rho} = \frac{\delta \rho}{\rho} - 3H \frac{\delta q}{\dot{\rho}}, \quad (6.129)$$

where $\delta \rho_m$ is defined by Eq. (6.69). Eliminating the term $\psi' - \mathcal{H}\mathcal{A}$ from Eqs. (6.97) and (6.98) of the fluid and using the gauge-invariant quantities Φ and δ_m , we obtain the Poisson equation

$$\nabla^2 \Phi + 3\mathcal{K}\Phi = -4\pi G a^2 \rho \delta_m. \quad (6.130)$$

The same equation also follows from Eqs. (6.114) and (6.115) of the scalar field.

A gauge-invariant sound speed $\hat{c}_s^2$ can be constructed by setting $\delta\hat{s} = (\hat{c}_s^2 - c_a^2)\delta_m$ in Eq. (6.128). Then, it follows that

$$\hat{c}_s^2 = \frac{\delta P - 3Hc_a^2\delta q}{\delta\rho - 3H\delta q}. \quad (6.131)$$

In the fluid rest frame ($\delta q = 0$), the gauge-invariant sound speed squared (6.131) reduces to $\hat{c}_s^2 = \delta P/\delta\rho$. For the perfect fluid, this rest-frame sound speed squared is equivalent to c_a^2 , whereas, for the imperfect fluid, $\hat{c}_s^2 \neq c_a^2$.

For the scalar field given by the Lagrangian density $P(\phi, X)$, the field rest frame corresponds to $\delta\phi = 0$ from Eq. (6.62). Setting $\delta\phi = 0$ in Eqs. (6.57) and (6.59), the rest-frame sound speed squared reads

$$\hat{c}_s^2 = \frac{P_{,X}}{P_{,X} + 2XP_{,XX}}. \quad (6.132)$$

For the canonical scalar field ϕ given by the Lagrangian density $P = X - V(\phi)$ we have $\hat{c}_s^2 = 1$. For $P(\phi, X)$ containing non-linear functions in X , $\hat{c}_s^2$ generally differs from 1.

Let us consider the case in which the scalar-field action depends on X alone [13], i.e.,

$$S = \int d^4x \sqrt{-g} P(X). \quad (6.133)$$

On using the fact that the background field density is given by $\rho = 2XP_{,X} - P$, the adiabatic sound speed squared $\hat{c}_a^2 = \dot{P}/\dot{\rho}$ reduces to

$$c_a^2 = \frac{P_{,X}}{P_{,X} + 2XP_{,XX}}, \quad (6.134)$$

which is the same as Eq. (6.132). This means that, as long as scalar perturbations are concerned, the theory (6.133) can describe the perfect fluid for the time-dependent FLRW background (characterized by a time-like vector field $\partial_\mu\phi$ satisfying $X > 0$) [14, 15].

If the Lagrangian density $P(\phi, X)$ contains the dependence of both ϕ and X , then the adiabatic sound speed squared is different from Eq. (6.134). Hence, in this case, the scalar field behaves as an imperfect fluid.

6.7. Second-order perturbed actions in the presence of a scalar field

So far, we have derived the equations of linear cosmological perturbations by perturbing the Einstein equation (3.85). Another way of the derivation is to expand the action of a given theory up to second order in perturbations. This method is powerful for finding no ghost and stability conditions of dynamical degrees of freedom even for theories beyond the framework of GR (as we will see in Chaps. 12 and 13). Moreover,

it is useful for identifying a canonical scalar field associated with a quantization procedure (as we will see in Sec. 6.8). In this section, we perform a second-order expansion of the action described by the system of a single canonical scalar field ϕ with a potential $V(\phi)$, i.e.,

$$S = \int d\eta d^3x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} R - \frac{1}{2} g^{\mu\nu} \nabla_\mu \phi \nabla_\nu \phi - V(\phi) \right]. \quad (6.135)$$

After deriving the second-order perturbed actions of Eq. (6.135), we can apply them to the computations of primordial power spectra generated during inflation. We will do so in Sec. 6.8 for probing observational signatures of inflation.

6.7.1. Background equations

Expanding the action (6.135) up to linear order in scalar perturbations, it is possible to derive the background equations of motion on the FLRW spacetime. Let us consider the flat expanding background ($\mathcal{K} = 0$) with the line element

$$ds^2 = a^2(\eta) [-N^2(\eta) d\eta^2 + a^2(\eta) \delta_{ij} dx^i dx^j], \quad (6.136)$$

where $N(\eta)$ is a time-dependent function called the lapse. Expanding the action (6.135) for the metric (6.136) and varying it with respect to N, a, ϕ , we can derive the background equations of motion. In the language of the perturbed metric (6.13), this amounts to considering the time-dependent functions $A(\eta)$ and $\psi(\eta)$ together with the time-dependent field perturbation $\delta\phi(\eta)$. Dealing with $A, \psi, \delta\phi$ as space-independent perturbations and expanding the action (6.135) up to first order in A, ψ , and $\delta\phi$, we obtain the first-order action $S^{(1)} = \int d\eta d^3x L^{(1)}$, where

$$\begin{aligned} L^{(1)} = & -\frac{1}{2} a^2 (6M_{\text{pl}}^2 \mathcal{H}^2 + 6M_{\text{pl}}^2 \mathcal{H}' + \phi'^2 + 2a^2 V) A - 3M_{\text{pl}}^2 a^2 \mathcal{H} A' \\ & + \frac{3}{2} a^2 (6M_{\text{pl}}^2 \mathcal{H}^2 + 6M_{\text{pl}}^2 \mathcal{H}' + \phi'^2 - 2a^2 V) \psi + 3M_{\text{pl}}^2 a^2 (\psi'' + 3\mathcal{H}\psi') \\ & + a^2 \phi' \delta\phi' - a^4 V_{,\phi} \delta\phi. \end{aligned} \quad (6.137)$$

After integrating the derivative terms $A', \psi', \psi'', \delta\phi'$ by parts, the Lagrangian $L^{(1)}$ reduces to

$$\begin{aligned} L^{(1)} = & a^2 \left(3M_{\text{pl}}^2 \mathcal{H}^2 - \frac{1}{2} \phi'^2 - a^2 V \right) A + \frac{3}{2} a^2 [2M_{\text{pl}}^2 (2\mathcal{H}' + \mathcal{H}^2) + \phi'^2 - 2a^2 V] \psi \\ & - a^2 (\phi'' + 2\mathcal{H}\phi' + a^2 V_{,\phi}) \delta\phi, \end{aligned} \quad (6.138)$$

up to boundary terms. Varying the action $S^{(1)}$ with respect to $A, \psi, \delta\phi$, we obtain

$$3M_{\text{pl}}^2 \mathcal{H}^2 = \frac{1}{2} \phi'^2 + a^2 V, \quad (6.139)$$

$$2M_{\text{pl}}^2 (\mathcal{H}' - \mathcal{H}^2) = -\phi'^2, \quad (6.140)$$

$$\phi'' + 2\mathcal{H}\phi' + a^2 V_{,\phi} = 0. \quad (6.141)$$

The second equation follows by combining two equations derived after the variations of A and ψ . We can easily confirm that Eqs. (6.139)–(6.141) agree with Eqs. (4.96)–(4.98), respectively.

6.7.2. Second-order action of scalar perturbations

For the computation of the second-order action of scalar perturbations, we first fix gauge degrees of freedom associated with the transformation (6.16). We choose the comoving (unitary) gauge where the scalar-field perturbation vanishes, i.e.,

$$\delta\phi = 0, \quad (6.142)$$

so that the temporal component ξ^0 of the gauge-transformation vector ξ^μ is fixed. To fix the spatial scalar component ξ of ξ^μ , we also choose the gauge $E = 0$. Since vector perturbations do not have a growing mode for the scalar-field theory (6.135), we consider only scalar and tensor perturbations on the flat FLRW background. We also note that, under the gauge choice (6.142), the comoving curvature perturbation $\mathcal{R}$ defined by Eq. (6.68) is equivalent to ψ . Then, the perturbed line element (6.13) for scalar perturbations is given by

$$ds^2 = a^2(\eta) \{ -(1 + 2A)d\eta^2 + 2B_{|i}d\eta dx^i + (1 + 2\mathcal{R})\delta_{ij}dx^i dx^j \}. \quad (6.143)$$

Expanding the action (6.135) up to second order in perturbations and integrating it by parts, the second-order scalar action yields

$$\begin{aligned} S_s^{(2)} = \int d\eta d^3x a^2 [& -3M_{\text{pl}}^2 \mathcal{R}'^2 + 2M_{\text{pl}}^2 \mathcal{R}' \partial^2 B - 2M_{\text{pl}}^2 \mathcal{H} A \partial^2 B + M_{\text{pl}}^2 (\partial \mathcal{R})^2 \\ & - 2M_{\text{pl}}^2 A \partial^2 \mathcal{R} + 6M_{\text{pl}}^2 \mathcal{H} A \mathcal{R}' - \frac{1}{2} (6\mathcal{H}^2 M_{\text{pl}}^2 - \phi'^2) A^2], \end{aligned} \quad (6.144)$$

where $(\partial \mathcal{R})^2 \equiv (\partial_{x_1} \mathcal{R})^2 + (\partial_{x_2} \mathcal{R})^2 + (\partial_{x_3} \mathcal{R})^2$ with the operators $\partial_{x_1} \equiv \partial/\partial x_1$ and $\partial^2 \equiv \partial_{x_1}^2 + \partial_{x_2}^2 + \partial_{x_3}^2$. We note that the terms like $\mathcal{R}^2$ and $\mathcal{R}A$ vanish on account of the background equations of motion (6.139)–(6.141). Variations with respect to A and B lead, respectively, to

$$(\phi'^2 - 6M_{\text{pl}}^2 \mathcal{H}^2) A + 2M_{\text{pl}}^2 (3\mathcal{H}\mathcal{R}' - \partial^2 \mathcal{R}) = 2M_{\text{pl}}^2 \mathcal{H} \partial^2 B, \quad (6.145)$$

$$\mathcal{H}A = \mathcal{R}', \quad (6.146)$$

where, for the derivation of Eq. (6.146), we have set the integration constant 0. We can confirm that Eqs. (6.145) and (6.146) agree with Eqs. (6.114) and (6.115), respectively. Substituting Eq. (6.146) into Eq. (6.144), the terms containing $\partial^2 B$ cancel each other. The term $c(\eta)\mathcal{R}'\partial^2 \mathcal{R}$, where $c(\eta)$ is an arbitrary function of η , is

equivalent to $c'(\eta)(\partial\mathcal{R})^2/2$ up to a boundary term. Then, the action (6.144) finally reduces to

$$S_s^{(2)} = \int d\eta d^3x a^2 Q_s [\mathcal{R}'^2 - c_s^2 (\partial\mathcal{R})^2], \quad (6.147)$$

where

$$Q_s \equiv \frac{\phi'^2}{2\mathcal{H}^2}, \quad c_s^2 = 1. \quad (6.148)$$

The result (6.147) shows that there is only one propagating scalar degree of freedom $\mathcal{R}$. The sign of Q_s in front of the kinetic term $\mathcal{R}'^2$ determines the no-ghost condition of scalar perturbations. Provided that $Q_s > 0$, which is the case for the present theory, the scalar ghost is absent. The quantity c_s corresponds to the scalar propagation speed, which is equivalent to the speed of light for the theory under consideration. As we will see in Sec. 10.2, in k-essence described by the action (6.54), the propagation speed squared (6.132) appears in front of the term $(\partial\mathcal{R})^2$ in Eq. (6.147). Varying the action (6.147) with respect to $\mathcal{R}$, the equation of motion for curvature perturbations is

$$\mathcal{R}'' + \frac{(a^2 Q_s)'}{a^2 Q_s} \mathcal{R}' - c_s^2 \partial^2 \mathcal{R} = 0. \quad (6.149)$$

To discuss the dynamics of scalar perturbations, we just need to solve Eq. (6.149) on a given cosmological background. We expand $\mathcal{R}$ in terms of the Fourier modes as

$$\mathcal{R}(\eta, \mathbf{x}) = \frac{1}{(2\pi)^3} \int d^3\mathbf{k} \mathcal{R}_k(\eta, \mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (6.150)$$

where $\mathbf{k}$ is a comoving wave number. Then, each Fourier mode satisfies

$$\mathcal{R}_k'' + \frac{(a^2 Q_s)'}{a^2 Q_s} \mathcal{R}_k' + c_s^2 k^2 \mathcal{R}_k = 0. \quad (6.151)$$

The Laplacian instability on small scales (large k) can be avoided for $c_s^2 > 0$. In Sec. 6.8, we will derive the scalar power spectrum generated during inflation by solving Eq. (6.151).

In modified gravitational theories discussed later in Chaps. 11–13, there are cases in which Q_s and c_s^2 become negative. For the theoretical consistency, we require the two conditions $Q_s > 0$ and $c_s^2 > 0$.

6.7.3. Second-order action of tensor perturbations

Let us next proceed to the derivation of the second-order action of tensor perturbations on the flat FLRW background. The line element for the tensor sector is

given by

$$ds^2 = a^2(\eta) \{-d\eta^2 + (\delta_{ij} + h_{ij})dx^i dx^j\}. \quad (6.152)$$

As we already mentioned, the tensor perturbation h_{ij} has two polarization states h_+ and $h_\times$. We can express h_{ij} in the form

$$h_{ij} = h_+ e_{ij}^+ + h_\times e_{ij}^\times, \quad (6.153)$$

where two polarization tensors e_{ij}^+ and $e_{ij}^\times$ are symmetric, divergence-free, traceless, and obey the normalization conditions

$$e_{ij}^+(\mathbf{k}) e_{ij}^\times(-\mathbf{k})^* = 0, \quad e_{ij}^\lambda(\mathbf{k}) e_{ij}^\lambda(-\mathbf{k})^* = 2, \quad (6.154)$$

for each $\lambda = +, \times$. For practical computations of the second-order action of tensor perturbations, we can consider gravitational waves propagating in the z -direction with spatial metric tensors:

$$\begin{aligned} g_{11} &= a^2(\eta) [1 + h_+(\eta, z)], & g_{22} &= a^2(\eta) [1 - h_+(\eta, z)], \\ g_{12} &= g_{21} = a^2(\eta) h_\times(\eta, z), & g_{33} &= a^2(\eta), \end{aligned} \quad (6.155)$$

where h_+ and $h_\times$ depend on η and z alone. These tensor modes obey the divergence-free and traceless conditions given by Eqs. (6.11) and (6.12).

Expanding the action (6.135) up to second order in tensor perturbations, integrating it by parts, and using the background equations of motion (6.139)–(6.141), the second-order tensor action yields

$$S_t^{(2)} = \sum_{\lambda=+, \times} \int d\eta d^3x a^2 Q_t [h_\lambda'^2 - c_t^2 (\partial h_\lambda)^2], \quad (6.156)$$

where

$$Q_t = \frac{M_{\text{pl}}^2}{4}, \quad c_t^2 = 1. \quad (6.157)$$

This means that, for the theory given by the action (6.135), the two tensor polarization modes propagate with the speed of light ($c_t = 1$). The quantity Q_t is positive, so there is no tensor ghost for the theory under consideration. The equation of motion following from the variation of (6.156) reads

$$h_\lambda'' + 2\mathcal{H}h_\lambda' - \partial^2 h_\lambda = 0, \quad (6.158)$$

which is used for the computation of the tensor power spectrum generated during inflation in Sec. 6.8.

6.8. Primordial power spectra generated during inflation

In this section, we derive the power spectra of scalar and tensor perturbations generated during inflation for the model given by the action (6.135). As we already discussed in Sec. 4.6, the perturbations inside the Hubble radius ($k > aH$) at the onset of inflation are causally connected. During inflation, the causally connected regions are stretched out over the Hubble radius ($k < aH$). Initially the perturbations exhibit damped oscillations as quantum vacuum fluctuations, but they start to behave as classical waves after the gravitational effect manifests itself for $k \lesssim aH$. We study the evolution of scalar and tensor perturbations before and after the Hubble radius crossing.

6.8.1. Scalar power spectrum

We first decompose the curvature perturbation $\mathcal{R}(\eta, \mathbf{x})$ in the form (6.150) with Fourier components:

$$\mathcal{R}_k(\eta, \mathbf{k}) = u(\eta, \mathbf{k})a(\mathbf{k}) + u^*(\eta, -\mathbf{k})a^\dagger(-\mathbf{k}), \quad (6.159)$$

where $a(\mathbf{k})$ and $a^\dagger(\mathbf{k})$ are annihilation and creation operators, respectively, obeying the commutation relations

$$[a(\mathbf{k}_1), a^\dagger(\mathbf{k}_2)] = (2\pi)^3 \delta^{(3)}(\mathbf{k}_1 - \mathbf{k}_2), \quad (6.160)$$

$$[a(\mathbf{k}_1), a(\mathbf{k}_2)] = [a^\dagger(\mathbf{k}_1), a^\dagger(\mathbf{k}_2)] = 0. \quad (6.161)$$

In quantum field theory, the vacuum state $|0\rangle$ is defined according to the condition

$$a(\mathbf{k})|0\rangle = 0. \quad (6.162)$$

From Eq. (6.151), each Fourier mode $u(\eta, \mathbf{k})$ obeys

$$u'' + \frac{(a^2 Q_s)'}{a^2 Q_s} u' + k^2 u = 0, \quad (6.163)$$

where we used $c_s^2 = 1$ for the model (6.135). Introducing the variables

$$v = zu, \quad z = a\sqrt{2Q_s} = \frac{a\phi'}{\mathcal{H}}, \quad (6.164)$$

we can write Eq. (6.163) in the form

$$v'' + \left(k^2 - \frac{z''}{z}\right)v = 0. \quad (6.165)$$

The conformal time $\eta = \int a^{-1} dt$ can be expressed as

$$\eta = \int \frac{da}{a^2 H} = -\frac{1}{aH} + \int \epsilon \frac{da}{a^2 H}, \quad (6.166)$$

where $\epsilon = -\dot{H}/H^2$. During inflation, the slow-roll parameter ϵ stays nearly constant with $\epsilon \ll 1$. Then, we have the approximate relation $\eta \simeq -(1 + \epsilon)/(aH)$. The asymptotic past ($a \rightarrow 0$) and the future ($a \rightarrow \infty$) correspond to $\eta \rightarrow -\infty$ and $\eta \rightarrow -0$, respectively. From Eqs. (4.100) and (4.102) the slow-roll parameter is approximately given by $\epsilon \simeq \dot{\phi}^2/(2M_{\text{pl}}^2 H^2)$, so Q_s can be expressed as $Q_s \simeq \epsilon M_{\text{pl}}^2$. Then the variation of Q_s during inflation is small, such that $\delta_{Q_s} \equiv \dot{Q}_s/(H Q_s)$ can be regarded as a small parameter much less than 1. Then, the quantity z''/z in Eq. (6.165) is estimated as

$$\frac{z''}{z} = 2(aH)^2 \left(1 - \frac{1}{2}\epsilon + \frac{3}{4}\delta_{Q_s} \right) + \mathcal{O}(\epsilon^2). \quad (6.167)$$

In the asymptotic past ($k\eta \rightarrow -\infty$), we have $k^2 \gg |z''/z|$ and hence $k \gg aH$. In this regime, Eq. (6.165) is approximately given by

$$v'' + k^2 v \simeq 0. \quad (6.168)$$

In terms of the quantity v , the kinetic term in the second-order action (6.147) is expressed as $\int d\eta d^3x v'^2/2$. This means that the perturbation v is a canonical scalar field that should be quantized. In the quantum field theory of curved spacetime, we can choose the so-called Bunch-Davies vacuum with a zero occupation number of particles [16]. This vacuum state corresponds to

$$v = \frac{e^{-ik\eta}}{\sqrt{2k}} = \frac{e^{-ik\eta}}{\sqrt{2k}}, \quad (6.169)$$

so the field v exhibits zero-point oscillations for $k\eta \rightarrow -\infty$.

Since the quantity $z''/z \simeq 2(aH)^2$ increases during inflation, this term becomes comparable to k^2 around the Hubble radius crossing ($k = aH$). Due to the gravitational effect induced by the term z''/z , the perturbation starts to grow for $k \lesssim aH$. In the de Sitter limit characterized by constant H , we have $\eta = -1/(aH)$ and hence $z''/z = 2/\eta^2$ in Eq. (6.167). Then, the solution to Eq. (6.165) can be expressed as

$$v = -\frac{\sqrt{\pi|\eta|}}{2} \left[c_1 H_{3/2}^{(1)}(x) + c_2 H_{3/2}^{(2)}(x) \right], \quad (6.170)$$

where $x = k|\eta|$, $c_{1,2}$ are integration constants, and $H_{3/2}^{(1)}(x) = -\sqrt{2}(1+i/x)e^{ix}/\sqrt{\pi x}$, $H_{3/2}^{(2)}(x) = (H_{3/2}^{(1)}(x))^*$ are Hankel functions of the first and second kinds with index $\nu = 3/2$. To recover the solution (6.169) in the limit $x \rightarrow \infty$, the coefficients in Eq. (6.170) are fixed as $c_1 = 1$ and $c_2 = 0$. Then, the resulting solution to $u = v/(a\sqrt{2Q_s})$ is given by

$$u(\eta, k) = \frac{i H e^{-ik\eta}}{2k^{3/2}\sqrt{Q_s}} (1 + ik\eta). \quad (6.171)$$

If we take into account the deviation from the exact de Sitter background, the solution (6.171) is subject to modifications. However, the correction to the leading-order scalar power spectrum is of the order of ϵ [17], so it is a good approximation to neglect the variation of H .

Long after the Hubble radius crossing ($k\eta \ll 1$), the perturbation u approaches the value

$$u(0, k) = \frac{iH}{2k^{3/2}\sqrt{Q_s}}. \quad (6.172)$$

Since u is nearly frozen after the Hubble radius crossing, the value (6.172) can be well approximated as that at $k = aH$. For a vacuum state $|0\rangle$, the two-point correlation function of curvature perturbations for $\eta \rightarrow 0$ is given by the vacuum expectation value $\langle 0|\mathcal{R}_k(0, \mathbf{k}_1)\mathcal{R}_k(0, \mathbf{k}_2)|0\rangle$. We define the power spectrum $P_{\mathcal{R}}$ of curvature perturbations, as

$$\langle 0|\mathcal{R}_k(0, \mathbf{k}_1)\mathcal{R}_k(0, \mathbf{k}_2)|0\rangle = P_{\mathcal{R}}(k_1) (2\pi)^3 \delta^{(3)}(\mathbf{k}_1 + \mathbf{k}_2), \quad (6.173)$$

where $\delta^{(3)}(\mathbf{x})$ is the three-dimensional delta function. On using Eqs. (6.159)–(6.161), it follows that $P_{\mathcal{R}}(k) = |u(0, k)|^2$. From Eq. (6.172), we obtain

$$P_{\mathcal{R}}(k) = \frac{H^2}{4Q_s k^3} \Big|_{k=aH}, \quad (6.174)$$

where we have employed the approximation that $u(0, k)$ is equivalent to the value u at $k = aH$. The vacuum expectation value of $P_{\mathcal{R}}(k)$ integrated in terms of comoving wave numbers k is given by

$$\langle \mathcal{R}^2 \rangle = \frac{1}{(2\pi)^3} \int d^3\mathbf{k} P_{\mathcal{R}}(k) = \frac{1}{2\pi^2} \int dk k^2 P_{\mathcal{R}}(k). \quad (6.175)$$

Introducing the quantity $\mathcal{P}_{\mathcal{R}}(k) \equiv k^3 P_{\mathcal{R}}(k)/(2\pi^2)$, we can express $\langle \mathcal{R}^2 \rangle$ in the form $\langle \mathcal{R}^2 \rangle = \int d \ln k \mathcal{P}_{\mathcal{R}}(k)$. In the context of inflationary cosmology, the quantity $\mathcal{P}_{\mathcal{R}}(k)$ is often called the power spectrum [17–19]. In this case, we have

$$\mathcal{P}_{\mathcal{R}}(k) = \frac{k^3}{2\pi^2} P_{\mathcal{R}}(k) = \frac{H^2}{8\pi^2 Q_s} \Big|_{k=aH} = \frac{H^2}{8\pi^2 M_{\text{pl}}^2 \epsilon} \Big|_{k=aH}, \quad (6.176)$$

which should be evaluated at $k = aH$. The result (6.176) has been derived for the unitary gauge (6.142), but the same power spectrum also follows for other gauge choices like the Newtonian gauge (6.73).

Under the slow-roll approximation discussed in Sec. 4.6, we have $H^2 \simeq V/(3M_{\text{pl}}^2)$ and $\epsilon \simeq \epsilon_V = (M_{\text{pl}}^2/2)(V_{,\phi}/V)^2$. Then, the power spectrum (6.176) can

be expressed as

$$\mathcal{P}_{\mathcal{R}}(k) = \frac{V^3}{12\pi^2 M_{\text{pl}}^6 V_{,\phi}^2} \Big|_{k=aH}. \quad (6.177)$$

Since H is nearly constant during inflation, the perturbations with larger k cross the Hubble radius at later epochs. Hence the power spectrum (6.177) depends on the wave number k . To quantify this scale dependence, we define the scalar spectral index n_s , as

$$n_s - 1 \equiv \frac{d \ln \mathcal{P}_{\mathcal{R}}(k)}{d \ln k} \Big|_{k=aH}. \quad (6.178)$$

At the Hubble radius crossing, we have the approximate relation $d \ln k \simeq d \ln a = H dt$, where we used the fact that H is nearly constant. Then, the scalar spectral index for the power spectrum (6.177) reads

$$n_s - 1 = \frac{\dot{\mathcal{P}}_{\mathcal{R}}}{H \mathcal{P}_{\mathcal{R}}} = \frac{3V_{,\phi}\dot{\phi}}{H V} - \frac{2V_{,\phi\phi}\dot{\phi}}{H V_{,\phi}}. \quad (6.179)$$

Employing the slow-roll approximations (4.100) and (4.101), it follows that

$$n_s - 1 = -6\epsilon_V + 2\eta_V, \quad (6.180)$$

where ϵ_V and η_V are slow-roll parameters defined by Eq. (4.103). Since $\{\epsilon_V, |\eta_V|\} \ll 1$ during inflation, the spectral index n_s is close to 1. For $n_s = 1$, the power spectrum is given by $\mathcal{P}_{\mathcal{R}} \propto k^{n_s-1} = k^0$, so it does not depend on the scale (called scale-invariant). Thus, the inflationary paradigm generates the nearly scale-invariant power spectrum of scalar perturbations. Although the deviation of n_s from 1 is small, it is possible to distinguish between different inflationary models from the observations of CMB temperature anisotropies (as we will see in Sec. 6.8.3). The power spectra with $n_s < 1$ and $n_s > 1$ are called red-tilted and blue-tilted, respectively.

If we ignore the scale dependence of n_s , the power spectrum can be expanded around a pivot wave number k_0 , as

$$\mathcal{P}_{\mathcal{R}}(k) = \mathcal{P}_{\mathcal{R}}(k_0) \left(\frac{k}{k_0} \right)^{n_s-1}. \quad (6.181)$$

To allow the scale dependence of n_s , we introduce the running of n_s , as

$$\alpha_s \equiv \frac{dn_s}{d \ln k} \Big|_{k=aH}. \quad (6.182)$$

We employ the relations $\dot{\epsilon}_V/H = -2\epsilon_V\eta_V + 4\epsilon_V^2$ and $\dot{\eta}_V/H = 2\epsilon_V\eta_V - \xi_V^2$, where

$$\xi_V^2 \equiv \frac{M_{\text{pl}}^4 V_{,\phi} V_{,\phi\phi\phi}}{V^2}. \quad (6.183)$$

Then, Eq. (6.182) becomes

$$\alpha_s = 16\epsilon_V\eta_V - 24\epsilon_V^2 - 2\xi_V^2, \quad (6.184)$$

which is of second order in slow-roll parameters. Taking into account the scalar running α_s , the power spectrum can be further expanded as

$$\ln \mathcal{P}_{\mathcal{R}}(k) = \ln \mathcal{P}_{\mathcal{R}}(k_0) + [n_s(k_0) - 1]y + \frac{\alpha_s(k_0)}{2}y^2 + \mathcal{O}(y^3), \quad (6.185)$$

where $y = \ln(k/k_0)$. Provided that $|\alpha_s(k_0)y^2/2| \ll |[n_s(k_0) - 1]y|$, the terms higher than the order of y^2 can be neglected.

6.8.2. Tensor power spectrum

Let us next proceed to the derivation of the tensor power spectrum generated during inflation. The tensor perturbations h_λ , which have two polarization modes $\lambda = +, \times$, obey Eq. (6.122) in real space. In Fourier space, this equation translates to

$$h''_\lambda + 2\mathcal{H}h'_\lambda + k^2h_\lambda = 0, \quad (6.186)$$

on the flat FLRW background. From the second-order tensor action (6.156), the canonical field associated with h_λ is given by

$$v_t = z_t h_\lambda, \quad (6.187)$$

where $z_t = a\sqrt{2Q_t}$. Then, Eq. (6.186) reduces to

$$v''_t + \left(k^2 - \frac{z''_t}{z_t}\right)v_t = 0. \quad (6.188)$$

We can derive the solution to this equation by following the similar procedure to that for scalar perturbations. The solution to h_λ , which recovers the Bunch–Davies vacuum in the asymptotic past ($k\eta \rightarrow -\infty$), is given by

$$h_\lambda(\eta, k) = \frac{iH e^{-ik\eta}}{k^{3/2}M_{\text{pl}}} (1 + ik\eta). \quad (6.189)$$

On using the normalization conditions of e_{ij}^λ given by Eq. (6.154), the power spectrum of tensor perturbations after the Hubble radius crossing yields $\mathcal{P}_h(k) = 4 \cdot k^3 |h_\lambda(0, k)|^2 / (2\pi^2)$. Substituting the solution (6.189) with $k\eta \rightarrow 0$ into the expression of $\mathcal{P}_h(k)$, it follows that

$$\mathcal{P}_h(k) = \frac{2H^2}{\pi^2 M_{\text{pl}}^2} \Big|_{k=aH}, \quad (6.190)$$

which should be evaluated at $k = aH$. The tensor spectral index is given by

$$n_t \equiv \left. \frac{d \ln \mathcal{P}_h(k)}{d \ln k} \right|_{k=aH} = -2\epsilon \simeq -2\epsilon_V. \quad (6.191)$$

Since $\epsilon_V \ll 1$, the tensor power spectrum is close to scale invariant. We note, however, that there is a small deviation from the scale invariance, i.e., $n_t < 0$. This spectrum, which has a larger power for smaller k , is called a red-tilted spectrum. We also introduce the tensor running

$$\alpha_t \equiv \left. \frac{dn_t}{d \ln k} \right|_{k=aH} = -8\epsilon_V^2 + 4\epsilon_V \eta_V. \quad (6.192)$$

Around a pivot wave number k_0 , the tensor power spectrum can be expanded as

$$\ln \mathcal{P}_h(k) = \ln \mathcal{P}_h(k_0) + n_t(k_0)y + \frac{\alpha_t(k_0)}{2}y^2 + \mathcal{O}(y^3). \quad (6.193)$$

The terms higher than y^2 can be neglected for $|\alpha_t(k_0)y^2/2| \ll |n_t(k_0)y|$.

From Eqs. (6.176) and (6.190), the tensor-to-scalar ratio is given by

$$r \equiv \frac{\mathcal{P}_h}{\mathcal{P}_\mathcal{R}} = 16\epsilon. \quad (6.194)$$

Since $\epsilon \ll 1$ during inflation, the amplitude of tensor perturbations is suppressed relative to scalar perturbations. From Eqs. (6.191) and (6.194), we have

$$r = -8n_t, \quad (6.195)$$

which is called the consistency relation.

6.8.3. Observational constraints on inflationary models

When we confront inflationary models with CMB observations in terms of the power spectra (6.185) and (6.193), there are six observables $\mathcal{P}_\mathcal{R}(k_0)$, $n_s(k_0)$, $\alpha_s(k_0)$, $\mathcal{P}_h(k_0)$, $n_t(k_0)$, $\alpha_t(k_0)$. The runnings $\alpha_s(k_0)$ and $\alpha_t(k_0)$ are small under the slow-roll approximation, so the likelihood analysis can be performed by setting $\alpha_s(k_0) = 0 = \alpha_t(k_0)$. Since the consistency relation (6.195) holds between $r(k_0)$ and $n_t(k_0)$, the three parameters $\mathcal{P}_\mathcal{R}(k_0)$, $n_s(k_0)$, $r(k_0)$ are left in the analysis. The pivot wave numbers $k_0 = 0.002 \text{ Mpc}^{-1}$ and $k_0 = 0.05 \text{ Mpc}^{-1}$ are often used in the likelihood analysis of WMAP and Planck missions. The resulting observational constraints are not sensitive to the choice of pivot scales.

In 2015, the Planck mission temperature and polarization data on large angular scales constrained the three observables to be [20]

$$\ln(10^{10}\mathcal{P}_\mathcal{R}(k_0)) = 3.062 \pm 0.029 \quad (68\% \text{ CL}), \quad (6.196)$$

$$n_s(k_0) = 0.968 \pm 0.006 \quad (68\% \text{ CL}), \quad (6.197)$$

$$r(k_0) < 0.11 \quad (95\% \text{ CL}), \quad (6.198)$$

at $k_0 = 0.002 \text{ Mpc}^{-1}$. The observed scalar power spectrum is close to scale-invariant, but it is slightly red-tilted. Without setting the priors on the runnings, the Planck data constrained the scalar running to be $\alpha_s(k_0) = -0.003 \pm 0.007$ (68% CL), which is consistent with $\alpha_s(k_0) = 0$. On using Eq. (6.176), the Planck normalization (6.196) translates to

$$H(k_0) \simeq \sqrt{\epsilon(k_0)} \times 10^{15} \text{ GeV}. \quad (6.199)$$

For $\epsilon(k_0) = 0.01$, the energy scale of inflation is observationally constrained to be around 10^{14} GeV .

In Fig. 6.1, we show observational bounds in the (n_s, r) plane constrained from Planck 2013, WMAP polarization, and BAO data. On using these bounds, we can test for the viability of numerous inflationary models.

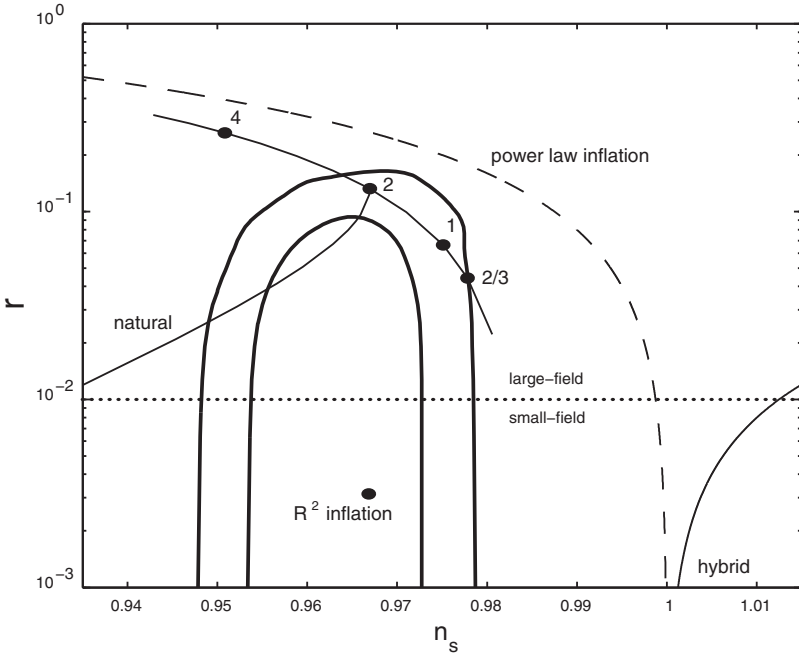


Fig. 6.1. Observational bounds on the scalar spectral index n_s and the tensor-to-scalar ratio r constrained from Planck 2013 [21], WMAP polarization [22], and BAO data [23–25] with the pivot wave number $k_0 = 0.05 \text{ Mpc}^{-1}$. Two thick lines represent 68% CL (inside) and 95% CL (outside) observational contours. We also plot theoretical predictions for the models (i) $V(\phi) = \lambda\phi^n/n$ with $n = 4, 2, 1, 2/3$, (ii) $V(\phi) = V_0 e^{-\lambda\phi/M_{\text{Pl}}}$ (“power-law inflation”), (iii) $V(\phi) = V_0[1 + \cos(\phi/f)]$ (“natural”), (iv) $V(\phi) = V_0 + m_\phi^2\phi^2/2$ with $V_0 \gg m_\phi^2\phi^2/2$ (“hybrid”), and (v) $f(R) = R + R^2/(6M^2)$ (“ R^2 inflation”). The number of e-foldings is fixed to be $\mathcal{N} = 60$ in all cases. The border between large-field and small-field models is characterized by the line $r \approx 10^{-2}$.

Let us first consider the chaotic inflationary scenario given by the potential (4.107). In this case, the slow-roll parameters are given by $\epsilon_V = n^2 M_{\text{pl}}^2 / (2\phi^2)$ and $\eta_V = n(n-1)M_{\text{pl}}^2 / \phi^2$, where ϕ is related to the number of e-foldings $\mathcal{N}$ as Eq. (4.108). From Eqs. (6.180) and (6.194), it follows that

$$n_s = 1 - \frac{2(n+2)}{4\mathcal{N}+n}, \quad r = \frac{16n}{4\mathcal{N}+n}. \quad (6.200)$$

For $\mathcal{N} = 60$, we have $n_s = 0.967$, $r = 0.132$ for $n = 2$ and $n_s = 0.951$, $r = 0.262$ for $n = 4$. The quartic potential ($n = 4$) is excluded at more than 99% CL. The quadratic potential ($n = 2$) is close to the border of 95% CL limit. By using the field value $\phi \simeq 15.6 M_{\text{pl}}$ at $\mathcal{N} = 60$ for the quadratic potential $V(\phi) = m_\phi^2 \phi^2 / 2$, the Planck normalization (6.196) with Eq. (6.177) constrains the mass scale to be $m_\phi \simeq 10^{13}$ GeV.

As we see in Sec. 10.1.2, the exponential potential $V(\phi) = V_0 e^{-\lambda\phi/M_{\text{pl}}}$ with $\lambda^2 < 2$ can lead to the power-law accelerated expansion characterized by $a \propto t^{2/\lambda^2}$. In this case we have $n_s - 1 = -\lambda^2$ and $r = 8\lambda^2$, so the model is on the line $r = 8(1 - n_s)$ in the (n_s, r) plane. As we see in Fig. 6.1, the power-law inflation is outside the 95% CL observational contour.

The potential (4.109) of natural inflation gives rise to smaller values of r relative to the quadratic potential $V(\phi) = m_\phi^2 \phi^2 / 2$. For a smaller symmetry breaking scale f , inflation occurs in the region closer to $\phi = 0$. Since n_s gets smaller for decreasing f , there is a lower observational bound $f \gtrsim 5M_{\text{pl}}$ constrained by the 95% CL contour in Fig. 6.1 [26].

There exists a so-called hybrid inflationary scenario [27] in which the inflaton field moves along the potential in the form $V(\phi) = V_0 + m_\phi^2 \phi^2 / 2$ by reaching a bifurcation point, after which the presence of another field χ gives rise to a “water-fall” transition towards a global minimum. Provided that $V_0 \gg m_\phi^2 \phi^2 / 2$, the scalar spectral index is estimated as $n_s - 1 \simeq 2\eta_V \simeq 2M_{\text{pl}}^2 m^2 / V_0 > 1$. This blue-tilted power spectrum is excluded from the Planck data.

In the Starobinsky model (4.111), the corresponding Einstein-frame action is given by Eq. (4.91) with the potential (4.112) of a scalar field (gravitational origin). In $f(R)$ gravity, inflationary observables in the Einstein frame are the same as those in the original frame (see Ref. [28] for details). On using the slow-roll parameters (4.114) and (4.115) with $\mathcal{N} \gg 1$, we obtain

$$n_s \simeq 1 - \frac{2}{\mathcal{N}}, \quad r \simeq \frac{12}{\mathcal{N}^2}. \quad (6.201)$$

For $\mathcal{N} = 60$ we have $n_s = 0.967$ and $r = 0.003$, in which case the model is well within the 68% CL observational contour shown in Fig. 6.1.

The tensor-to-scalar ratio r is related to the field variation $\Delta\phi = |\phi_{\text{CMB}} - \phi_{\text{end}}|$ during inflation, where ϕ_{CMB} and ϕ_{end} are the field values on scales observed in CMB measurements and at the end of inflation, respectively. Differentiating Eq. (4.106) with respect to $\mathcal{N}$, we obtain $(d\phi/d\mathcal{N})^2 = (M_{\text{pl}}^2/8)r$, where $r \simeq 8M_{\text{pl}}^2 (V_{,\phi}/V)^2$.

This gives the relation $\Delta\phi/M_{\text{pl}} = \int_{\mathcal{N}_{\text{end}}}^{\mathcal{N}_{\text{CMB}}} d\mathcal{N} \sqrt{r/8}$. As long as r does not vary much during inflation, the field variation can be estimated as

$$\frac{\Delta\phi}{M_{\text{pl}}} \simeq \mathcal{O}(1) \times \left(\frac{r}{0.01} \right)^{1/2}, \quad (6.202)$$

where we used the fact that $\mathcal{N}_{\text{CMB}} - \mathcal{N}_{\text{end}}$ is between 50 and 60. The relation (6.202) is called the Lyth bound [29]. The model with $\Delta\phi > M_{\text{pl}}$ is called a large-field model, in which case r is larger than the order of 0.01. Chaotic inflation is a representative model of this class. The model with $\Delta\phi < M_{\text{pl}}$ is called a small-field model, in which case $r < \mathcal{O}(0.01)$. Starobinsky inflation is a representative model of this class. In current CMB observations, only the upper limit of r has been constrained as Eq. (6.198), so we could not conclude yet whether small-field models are favored over large-field models or vice versa.

Existence of tensor perturbations leaves a peculiar rotational pattern called a B-mode on CMB temperature anisotropies [30]. If the B-mode were detected in future observations, the tensor-to-scalar ratio r can be tightly constrained. Then, we will be able to approach the best model of inflation. The B-mode detection measurements such as QUIET, POLARBEAR, LiteBIRD aim to reach the sensitivity of $r < \mathcal{O}(0.01)$.

6.9. Second-order action of perturbations in the presence of a perfect fluid

In Sec. 6.6, we observed that a time-like scalar field with a purely kinetic action (6.133) mimics a perfect fluid. This equivalence is helpful when we expand the corresponding action up to second order in scalar perturbations on the FLRW background. There is another description of the perfect fluid advocated by Schutz and Sorkin [31]. Unlike k-essence, this can not only accommodate the scalar propagation but also the vector propagation, so it is convenient to apply it to the theories containing dynamical degrees of freedom of vector perturbations. In Chap. 13, we will employ the Schutz–Sorkin action for generalized Proca theories with a massive vector field.

The Schutz–Sorkin action of the perfect fluid is given by

$$S_M = - \int d^4x [\sqrt{-g} \rho(n) + J^\mu (\partial_\mu \ell + \mathcal{A}_1 \partial_\mu \mathcal{B}_1 + \mathcal{A}_2 \partial_\mu \mathcal{B}_2)], \quad (6.203)$$

where the fluid density ρ is a function of its number density defined by

$$n = \sqrt{\frac{J^\alpha J^\beta g_{\alpha\beta}}{g}}. \quad (6.204)$$

The vector field J^μ and the scalar field ℓ describe scalar perturbations, whereas the scalar quantities $\mathcal{A}_{1,2}, \mathcal{B}_{1,2}$ are associated with vector perturbations. For the

covariant derivative of scalar quantities like ℓ , we adopt the notation like $\partial_\mu \ell$ instead of $\nabla_\mu \ell$ in the following. Variation of the matter action (6.203) leads to

$$u_\mu \equiv \frac{J_\mu}{n\sqrt{-g}} = \frac{1}{\rho_{,n}} (\partial_\mu \ell + \mathcal{A}_1 \partial_\mu \mathcal{B}_1 + \mathcal{A}_2 \partial_\mu \mathcal{B}_2), \quad (6.205)$$

where u_μ is the normalized four-velocity, and $\rho_{,n} \equiv \partial \rho / \partial n$.

We consider the flat FLRW background described by the line element $ds^2 = -dt^2 + a^2(t)(dx^2 + dy^2 + dz^2)$. Throughout this section, we use the cosmic time t instead of the conformal time η . On the isotropic and homogenous cosmological background, the vector contributions $\mathcal{A}_1 \partial_\mu \mathcal{B}_1 + \mathcal{A}_2 \partial_\mu \mathcal{B}_2$ should vanish. Since the temporal component u_0 is equivalent to -1 , it follows that $J^0 = -J_0 = n\sqrt{-g} = n_0(t)a^3(t)$ and $\partial_0 \ell = -\rho_{,n}(t)$, where $n_0(t)$ is the background fluid number density. On using the property $n_0(t) \propto a^{-3}(t)$, the total fluid number

$$\mathcal{N}_0 \equiv n_0(t)a^3(t) \quad (6.206)$$

is conserved. At the background level, the action (6.203) reduces to

$$S_M^{(0)} = \int d^4x \sqrt{-g} P, \quad P = n_0 \rho_{,n} - \rho, \quad (6.207)$$

where P corresponds to the pressure of the perfect fluid.

Let us consider perturbations on the flat FLRW background. First, we decompose temporal and spatial components of J^μ in the form

$$J^0 = \mathcal{N}_0 + \delta J, \quad (6.208)$$

$$J^i = \frac{1}{a^2(t)} \delta^{ik} (\partial_k \delta j + W_k), \quad (6.209)$$

where δJ and δj are scalar perturbations, and W_k is a vector perturbation obeying the transverse condition $\partial^k W_k = 0$. The scalar quantity ℓ is decomposed as

$$\ell = - \int^t \rho_{,n}(\tilde{t}) d\tilde{t} - \rho_{,n} \mathcal{V}, \quad (6.210)$$

where $\mathcal{V}$ is related to the velocity potential v discussed in Sec. 6.3.1 (as we will explicitly see below). From Eqs. (6.205) and (6.210), we find that the spatial component u_i originating from the scalar perturbation ℓ corresponds to $-\partial_i \mathcal{V}$.

For the vector mode, the simplest choice of $\mathcal{A}_1, \mathcal{A}_2, \mathcal{B}_1, \mathcal{B}_2$ keeping the required property of vector perturbations is given by [32]

$$\begin{aligned} \mathcal{A}_1 &= \delta \mathcal{A}_1(t, z), & \mathcal{A}_2 &= \delta \mathcal{A}_2(t, z), \\ \mathcal{B}_1 &= x + \delta \mathcal{B}_1(t, z), & \mathcal{B}_2 &= y + \delta \mathcal{B}_2(t, z), \end{aligned} \quad (6.211)$$

where $\delta \mathcal{A}_i$ and $\delta \mathcal{B}_i$ are perturbed quantities which depend on the time t and the third spatial component z . We also note that the vector field in the form

$W_k = (W_1(t, z), W_2(t, z), 0)$ obeys the transverse condition $\partial^k W_k = 0$. The intrinsic vector part $\mathcal{V}_i$ of the four velocity is related to the linear perturbation $\delta\mathcal{A}_i$, as

$$\delta\mathcal{A}_i = \rho_{,n}\mathcal{V}_i, \quad (6.212)$$

where $\mathcal{V}_i$ satisfies the transverse condition $\partial^i \mathcal{V}_i = 0$. From Eqs. (6.205), (6.210), (6.211) and (6.212), the spatial component of the four velocity is given by

$$u_i = -\partial_i \mathcal{V} + \mathcal{V}_i. \quad (6.213)$$

Compared to Eq. (6.38), we observe the following correspondences:

$$\mathcal{V} = -a(v + B), \quad (6.214)$$

$$\mathcal{V}_i = a(v_i - S_i). \quad (6.215)$$

The equation of motion for $\delta\mathcal{A}_i$ follows by expanding the action (6.203) up to second order in perturbations and by varying the action with respect to $\delta\mathcal{B}_i$. In Sec. 13.4.2, we will study the property of vector perturbations in more general theories where additional dynamical vector degrees of freedom like those originating from a Maxwell field stress tensor $F_{\mu\nu}$ are present.

In the rest of this section, we discuss how scalar perturbation equations of motion can be derived from the Schutz-Sorkin action (6.203) in the context of GR. Dropping the contribution of the vector sector, we expand the following action up to second order in scalar perturbations:

$$S = S_g + S_M, \quad (6.216)$$

where

$$S_g = \int d^4x \sqrt{-g} \frac{M_{\text{pl}}^2}{2} R, \quad S_M = - \int d^4x [\sqrt{-g} \rho(n) + J^\mu \partial_\mu \ell]. \quad (6.217)$$

For the gravity sector, we consider the linearly perturbed line-element

$$ds^2 = -(1 + 2\Psi) dt^2 + 2\partial_i \chi dt dx^i + a^2(t) (1 + 2\Phi) \delta_{ij} dx^i dx^j, \quad (6.218)$$

where Ψ, χ, Φ are scalar metric perturbations. For the metric (6.218), we have fixed the spatial scalar component of the gauge transformation vector ξ^μ , but the temporal component ξ^0 was not fixed. After Chap. 7, we will take several different gauges (like the Newtonian gauge $\chi = 0$, the flat gauge $\Phi = 0$, the unitary gauge $\delta\phi = 0$ in the presence of a scalar field ϕ), so it is convenient not to fix the temporal gauge for generality.

For the metric (6.218), we define the matter density perturbation, as

$$\delta\rho = \frac{\rho_{,n}}{a^3} (\delta J - 3\mathcal{N}_0 \Phi). \quad (6.219)$$

Then the perturbation of the fluid number density n , which is expanded up to second order, reads

$$\delta n = \frac{\delta \rho}{\rho, n} - \frac{\rho, n [\mathcal{N}_0^2 (\partial \chi)^2 + 2\mathcal{N}_0 \partial \chi \partial \delta j + (\partial \delta j)^2 + 3a^2 \mathcal{N}_0^2 \Phi^2] + 6a^5 \mathcal{N}_0 \Phi \dot{\nu} \delta \rho}{2\mathcal{N}_0 \rho, n a^5}. \quad (6.220)$$

At first order, δn is equivalent to $\delta \rho / \rho, n$. This consistency holds by defining $\delta \rho$ as Eq. (6.219). Expanding the matter action S_M in Eq. (6.216) in scalar perturbations, the second-order action yields

$$\begin{aligned} S_M^{(2)} = \int dt d^3 x \left\{ \frac{1}{2a^5 n_0 \rho, n^2} \left[\rho, n (\rho, n^2 (\partial \delta j)^2 + 2a^3 n_0 \rho, n^2 \partial \delta j \partial \mathcal{V} + 2a^8 n_0 \rho, n \dot{\nu} \delta \rho \right. \right. \\ \left. \left. - 6a^8 n_0^2 \rho, nn H \mathcal{V} \delta \rho) - a^8 n_0 \rho, nn \delta \rho^2 \right] - a^3 \Psi \delta \rho + \frac{\rho, n}{a^2} \partial \chi \partial \delta j \right. \\ \left. + \frac{3}{2} a^3 (n_0 \rho, n - \rho) \Phi^2 - 3a^3 \Phi \left(\rho \Psi + 3H n_0^2 \rho, nn \mathcal{V} - n_0 \rho, n \dot{\nu} \right) \right. \\ \left. + \frac{1}{2} a (n_0 \rho, n - \rho) (\partial \chi)^2 + \frac{1}{2} a^3 \rho \Psi^2 \right\}. \quad (6.221) \end{aligned}$$

Variation of this action with respect to δj leads to

$$\partial \delta j = -a^3 n_0 (\partial \mathcal{V} + \partial \chi). \quad (6.222)$$

On using this relation, we can eliminate the perturbation δj in Eq. (6.221) to give

$$\begin{aligned} S_M^{(2)} = \int dt d^3 x a^3 \left\{ \left(\dot{\nu} - 3H c_M^2 \mathcal{V} - \Psi \right) \delta \rho - \frac{c_M^2 \delta \rho^2}{2n_0 \rho, n} - \frac{n_0 \rho, n}{2a^2} [(\partial \mathcal{V})^2 + 2\partial \mathcal{V} \partial \chi] \right. \\ \left. + 3n_0 \rho, n \left(\dot{\nu} - 3H c_M^2 \mathcal{V} \right) \Phi + \frac{1}{2} \rho \Psi^2 - 3\rho \Psi \Phi - \frac{\rho}{2a^2} (\partial \chi)^2 + \frac{3}{2} P \Phi^2 \right\}, \quad (6.223) \end{aligned}$$

where $P = n_0 \rho, n - \rho$ is the pressure of the fluid, and c_M^2 corresponds to the matter sound speed squared given by

$$c_M^2 = \frac{P, n}{\rho, n} = \frac{n_0 \rho, nn}{\rho, n}. \quad (6.224)$$

The second-order action derived after the expansion of the Einstein-Hilbert action S_g in Eq. (6.216) is (up to boundary terms)

$$\begin{aligned} S_g^{(2)} = \int dt d^3 x a^3 M_{\text{pl}}^2 \left[\frac{2}{a^2} \left(\dot{\Phi} - H \Psi \right) \nabla^2 \chi - 3\dot{\Phi}^2 - \frac{2}{a^2} \Psi \partial^2 \Phi + \frac{(\partial \Phi)^2}{a^2} + 6H \Psi \dot{\Phi} \right. \\ \left. - \frac{9}{2} H^2 \Psi^2 + 9H^2 \Psi \Phi + \frac{3H^2}{2a^2} (\partial \chi)^2 + \frac{3}{2} \left(3H^2 + 2\dot{H} \right) \Phi^2 \right]. \quad (6.225) \end{aligned}$$

On using the background equations of motion $3M_{\text{pl}}^2 H^2 = \rho$ and $M_{\text{pl}}^2(3H^2 + 2\dot{H}) = -P$, the last three terms of Eqs. (6.223) and (6.225) cancel each other. Then, the total second-order action $S^{(2)} = S_M^{(2)} + S_g^{(2)}$ yields

$$\begin{aligned}
S^{(2)} = \int dt d^3x a^3 \Big\{ & \frac{2M_{\text{pl}}^2}{a^2} (\dot{\Phi} - H\Psi) \nabla^2 \chi - 3M_{\text{pl}}^2 H^2 \Psi^2 + \frac{M_{\text{pl}}^2 (\partial\Phi)^2}{a^2} - 3M_{\text{pl}}^2 \dot{\Phi}^2 \\
& + 2M_{\text{pl}}^2 \left(3H\dot{\Phi} - \frac{\partial^2 \Phi}{a^2} \right) \Psi - \Psi \delta\rho + \left(\dot{\mathcal{V}} - 3Hc_M^2 \mathcal{V} \right) (\delta\rho + 3n_{0\rho,n} \Phi) \\
& - \frac{c_M^2 \delta\rho^2}{2n_{0\rho,n}} - \frac{n_{0\rho,n}}{2a^2} [(\partial\mathcal{V})^2 + 2\partial\mathcal{V}\partial\chi] \Big\}. \tag{6.226}
\end{aligned}$$

The perturbation equations of motion follow by varying the action (6.226) with respect to $\Psi, \chi, \Phi, \mathcal{V}, \delta\rho$. They match with the scalar perturbation equations derived in Sec. 6.5.1 with the correspondences $A \rightarrow \Psi, B \rightarrow a^{-1}\chi, \psi \rightarrow \Phi, E \rightarrow 0, v + B \rightarrow -a^{-1}\mathcal{V}, \delta q = -(\rho + P)\mathcal{V}, \delta P \rightarrow c_M^2 \delta\rho, \Pi \rightarrow 0, \mathcal{H} \rightarrow aH, \rho + P \rightarrow n_{0\rho,n}$. Since we are considering the perfect fluid, the matter sound speed squared c_M^2 is equivalent to the adiabatic sound speed squared $\dot{P}/\dot{\rho}$. Variations with respect to $\mathcal{V}$ and $\delta\rho$ lead, respectively, to

$$\delta\rho + 3H(1 + c_M^2)\delta\rho + (\rho + P) \left[3\dot{\Phi} - \frac{\nabla^2}{a^2}(\mathcal{V} + \chi) \right] = 0, \tag{6.227}$$

$$\dot{\mathcal{V}} - \Psi - 3Hc_M^2 \mathcal{V} - \frac{c_M^2}{\rho + P} \delta\rho = 0, \tag{6.228}$$

which match with Eqs. (6.105) and (6.107), respectively. On using Eq. (6.228) to eliminate the $\delta\rho$ term in Eq. (6.226) and integrating the term $\dot{\mathcal{V}}\mathcal{V}$ by parts, the second-order action can be written as

$$\begin{aligned}
S^{(2)} = \int dt d^3x a^3 M_{\text{pl}}^2 \Big[& \frac{2}{a^2} (\dot{\Phi} - H\Psi) \nabla^2 \chi - 3H^2 \Psi^2 + \frac{(\partial\Phi)^2}{a^2} - 3\dot{\Phi}^2 \\
& + 2 \left(3H\dot{\Phi} - \frac{\partial^2 \Phi}{a^2} \right) \Psi \Big] + \mathcal{S}_M^{(2)}, \tag{6.229}
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{S}_M^{(2)} = \int dt d^3x a^3 (\rho + P) \Big[& \frac{\dot{\mathcal{V}}^2}{2c_M^2} - \frac{(\partial\mathcal{V})^2}{2a^2} + \frac{3}{2} \dot{H} \mathcal{V}^2 - \frac{1}{a^2} \partial\mathcal{V}\partial\chi \\
& + (\dot{\mathcal{V}} - 3Hc_M^2 \mathcal{V}) \left(3\Phi - \frac{\Psi}{c_M^2} \right) + \frac{\Psi^2}{2c_M^2} \Big]. \tag{6.230}
\end{aligned}$$

The matter action $\mathcal{S}_M^{(2)}$ contains the kinetic term $\dot{\mathcal{V}}^2$, such that the velocity potential $\mathcal{V}$ works as a dynamical scalar propagating degree of freedom.

The discussion given above is valid for GR in the presence of the perfect fluid. In modified gravity theories, the action S_g is subject to change, but as long as the perfect fluid is minimally coupled to gravity, we can employ the Schutz-Sorkin action in the same way as discussed above. As we will see in Sec. 12.3, the second-order action of perfect fluid is the same as Eq. (6.230) even in most general scalar-tensor theories with second-order equations of motion (Horndeski theories).

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Chapter 7

Physics of CMB Temperature Anisotropies

In Sec. 6.8, we derived the primordial power spectra of scalar and tensor perturbations generated during inflation. They are regarded as initial conditions of perturbations at the onset of the radiation era. The perturbations re-enter the Hubble radius again long after the end of inflation. After this re-entry, the perturbation of photons starts to oscillate with a frequency associated with the sound speed of a coupled photon–baryon fluid. The oscillations of photons are imprinted in CMB temperature anisotropies. After the onset of the matter-dominated epoch, the gravitational instability of primordial perturbations leads to the growth of inhomogeneities to form large-scale structures in the Universe. In this section, we study the evolution of cosmological perturbations from the radiation-dominated epoch to today, paying particular attention to the physics of CMB temperature anisotropies.

7.1. Recombination and decoupling epochs

The production of light nuclei like deuterium and helium occurred in the first few minutes of the Big Bang with the temperature around $0.1 \text{ MeV} \lesssim T \lesssim 10 \text{ MeV}$. After this Big Bang nucleosynthesis, the mass fraction of helium is about 25% of masses of the total nuclei (see e.g., Refs. [1, 2] for details). While other light elements up to lithium are also produced, their mass ratios are much smaller relative to that of helium. In terms of the mass fraction, the single proton constitutes about 75% of the total nuclei.

In this section, we study the epoch at which the single proton (p) captures the electron (e^-) to form an atom, i.e., hydrogen (H). This process is characterized by the interaction

$$p + e^- \leftrightarrow H + \gamma, \tag{7.1}$$

where γ is the photon. Since the ionization energy of hydrogen is 13.6 eV, the reaction (7.1) proceeds to the left for a photon energy E_γ larger than 13.6 eV. In this case, the proton remains as a single ionized state. For the photon with $E_\gamma < 13.6$ eV, the reaction (7.1) proceeds to the right and hence the hydrogen atom can be generated. From Eqs. (4.37) and (4.38), the average energy of a single photon is given by

$$\langle E_\gamma \rangle = \frac{\varepsilon}{n} = \frac{\pi^4}{30\zeta(3)} k_B T \simeq 2.7 k_B T. \quad (7.2)$$

The temperature at which $\langle E_\gamma \rangle$ is equivalent to 13.6 eV translates to $T = 5.8 \times 10^4$ K. Crudely speaking, the hydrogen atom started to be formed after the photon temperature dropped below 10^4 K in the expanding Universe. However, as we see in Fig. 2.2, the energy distribution of CMB photons is not uniform, so the estimation given above is not very accurate. In what follows, we carry out a more elaborate treatment for estimating the epoch of the hydrogen formation.

We define the epoch of recombination at which the number density of hydrogen (n_H) is equivalent to that of proton (n_p), i.e., $n_H = n_p$. We consider the situation in which the interaction (7.1) is in a state of thermal equilibrium with temperature T . Around the temperature 10 eV, protons, electrons, hydrogens behaved as non-relativistic particles. From Eq. (4.41), their number densities read

$$n_X = g_X \left(\frac{m_X T}{2\pi} \right)^{3/2} e^{-(m_X - \mu_X)/T}, \quad (7.3)$$

where $X = p, e, H$. The internal degrees of freedom for protons, electrons, hydrogens are given, respectively, by $g_p = 2$, $g_e = 2$, $g_H = 4$. From the conservation of chemical potentials, it follows that $\mu_p + \mu_e = \mu_H$. Let us derive the value $n_H/(n_p n_e)$ from Eq. (7.3). Approximating the ratio m_H/m_p to be 1, we obtain the so-called Saha ionization equation [3]

$$\frac{n_H}{n_p n_e} = \left(\frac{m_e T}{2\pi} \right)^{-3/2} e^{Q/T}, \quad (7.4)$$

where $Q = m_p + m_e - m_H = 13.6$ eV is the ionization energy of hydrogen.

We define the ionization rate of proton as

$$X_p \equiv \frac{n_p}{n_p + n_H}, \quad (7.5)$$

with which the left hand side of Eq. (7.4) can be expressed as $(1 - X_p)/(X_p n_e)$. The neutrality condition gives the relation $n_e = n_p$. Ignoring the contribution from helium for the total baryon number density n_b , we have $n_b = n_p + n_H$ and hence $n_e = n_p = n_b X_p = n_\gamma \eta_b X_p$. Here, η_b is the baryon-to-photon ratio defined by

Eq. (4.65). Setting $g_* = 2$ in Eq. (4.37), the photon number density is given by $n_\gamma = 2\zeta(3)T^3/\pi^2$. Then, it follows that

$$n_e = n_p = \frac{2\zeta(3)T^3}{\pi^2} \eta_b X_p. \quad (7.6)$$

In summary, we can write Eq. (7.4) in the form

$$\frac{1 - X_p}{X_p^2} = 4\zeta(3) \sqrt{\frac{2}{\pi}} \eta_b \left(\frac{T}{m_e} \right)^{3/2} e^{Q/T}, \quad (7.7)$$

where $\eta_b = 2.7 \times 10^{-8} \Omega_b^{(0)} h^2$ from Eq. (4.66). Since the electron mass is $m_e = 5.11 \times 10^5 \text{ eV}$, the right hand side of Eq. (7.7) is much smaller than 1 for the temperature $T \sim Q = 13.6 \text{ eV}$. The ionization rate X_p is close to 1 at this epoch. After the temperature drops below Q , the exponential term $e^{Q/T}$ in Eq. (7.7) begins to grow and X_p approaches 0 in the limit that $T \ll Q$. Since the recombination epoch corresponds to $X_p = 1/2$, the temperature T_{rec} at recombination obeys the relation $(T_{\text{rec}}/m_e)^{3/2} e^{Q/T_{\text{rec}}} = 8.8 \times 10^8$, where we used $\Omega_b^{(0)} h^2 = 0.02205$. The numerical solution to this equation is given by

$$T_{\text{rec}} = 0.324 \text{ eV} = 3760 \text{ K}, \quad (7.8)$$

which corresponds to the redshift $z_{\text{rec}} = 1380$. This temperature is smaller than the one derived by using the average energy of photons by one order of magnitude.

After the hydrogen atom starts to be formed, the number density of free electrons decreases. Let us consider the Thomson scattering between photons and electrons, i.e.,

$$\gamma + e^- \leftrightarrow \gamma + e^-. \quad (7.9)$$

With the decrease of the number density of free electrons, the scattering rate between photons and electrons gets smaller. We define the epoch at which the Thomson scattering rate Γ is equivalent to the Hubble expansion rate H as the decoupling of photons. After the decoupling, the photons freely stream to us, so we can observe the photons emitted from the last scattering surface. In the following, we estimate the temperature at the CMB decoupling epoch.

The rate of Thomson scattering is given by $\Gamma = n_e \sigma_T c$, where n_e is the electron number density, σ_T is the scattering cross section, and c is the speed of light. We recall that n_e depends on the temperature T according to the relation (7.6). On using today's photon number density $n_\gamma^{(0)} = 2\zeta(3)T_0^3/\pi^2 \simeq 4.105 \times 10^8 \text{ m}^{-3}$, the Thomson scattering rate yields

$$\Gamma = n_\gamma^{(0)} \eta_b \sigma_T c \left(\frac{T}{T_0} \right)^3 X_p(T). \quad (7.10)$$

The decoupling of CMB photons occurs in the matter-dominated epoch, so we ignore the contributions of radiation, dark energy, and spatial curvature in Eq. (4.78), i.e.,

$H \simeq H_0 \sqrt{\Omega_m^{(0)}} (1+z)^{3/2} = H_0 \sqrt{\Omega_m^{(0)}} (T/T_0)^{3/2}$. Then, the ratio between Γ and H is given by

$$\frac{\Gamma}{H} = \frac{n_\gamma^{(0)} \eta_b \sigma_{TC}}{H_0 \sqrt{\Omega_m^{(0)}}} \left(\frac{T}{T_0} \right)^{3/2} X_p(T). \quad (7.11)$$

At high temperature $\Gamma \gg H$, but Γ/H decreases in time. The temperature corresponding to the CMB decoupling epoch ($\Gamma = H$) obeys

$$\left(\frac{T_*}{T_0} \right)^{3/2} X_p(T_*) = \frac{H_0 \sqrt{\Omega_m^{(0)}}}{n_\gamma^{(0)} \eta_b \sigma_{TC}} \simeq 14.7 \frac{\sqrt{\Omega_m^{(0)}}}{h \Omega_b^{(0)}}, \quad (7.12)$$

where we used Eqs. (2.9), (4.66), and $\sigma_T = 6.65 \times 10^{-29} \text{ m}^2$. Here, $X_p(T_*)$ is the solution to Eq. (7.7), i.e.,

$$X_p(T_*) = \frac{\sqrt{1+4\mathcal{Y}} - 1}{2\mathcal{Y}}, \quad \mathcal{Y} = 4\zeta(3) \sqrt{\frac{2}{\pi}} \eta_b \left(\frac{T_*}{m_e} \right)^{3/2} e^{Q/T_*}. \quad (7.13)$$

Substituting the typical values $\Omega_m^{(0)} = 0.31$, $\Omega_b^{(0)} h^2 = 0.02205$, $h = 0.68$, $T_0 = 2.725 \text{ K} = 2.348 \times 10^{-4} \text{ eV}$ into Eq. (7.12), we obtain the CMB decoupling temperature as

$$T_* = 0.263 \text{ eV} = 3060 \text{ K}, \quad (7.14)$$

which corresponds to the redshift $z_* = 1120$.

In the above discussion, we have assumed that the interaction (7.1) is in a state of thermal equilibrium. After Γ drops below H , we cannot ignore the deviation from thermal equilibrium. If the effect of such a non-equilibrium process is taken into account, it follows that the ionization rate X_p is larger than the one derived from Eq. (7.7). The production of the hydrogen atom was delayed by this effect, so that the redshift at decoupling is around 1090. More concretely, there is the following fitting formula [4]

$$z_* = 1048(1 + 0.00124\omega_b^{-0.738})(1 + g_1\omega_m^{g_2}), \quad (7.15)$$

where

$$g_1 = \frac{0.0783\omega_b^{-0.238}}{1 + 39.5\omega_b^{0.763}}, \quad g_2 = \frac{0.560}{1 + 21.1\omega_b^{1.81}}, \quad (7.16)$$

with $\omega_b = \Omega_b^{(0)} h^2$ and $\omega_m = \Omega_m^{(0)} h^2 = (\Omega_b^{(0)} + \Omega_c^{(0)}) h^2$.

7.2. Perturbed energy–momentum tensor, Boltzmann equation

Prior to the recombination epoch, the electron was strongly coupled to the proton through the Coulomb scattering (7.1). Before the decoupling of photons, the photon and the electron were also strongly coupled with each other. Hence photon, proton, and electrons behaved like a single photon–baryon fluid. Besides photons and baryons, there were dark matter and neutrinos gravitationally coupled with each other. To study the dynamics of perturbations of each matter species, we need to solve perturbed Boltzmann equations for this coupled system [5].

To study the evolution of perturbations after the onset of the radiation era, we consider the perturbed line element in the Newtonian gauge on the flat FLRW background:

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu = a^2(\eta) [-(1 + 2\Psi)d\eta^2 + (1 + 2\Phi)\delta_{ij}dx^i dx^j]. \quad (7.17)$$

This corresponds to the gauge choice $\tilde{B} = 0 = \tilde{E}$ in the line element (6.27). Under the gauge transformation $\tilde{x}^\mu = x^\mu + \xi^\mu$, the perturbations B and E are transformed as Eqs. (6.30) and (6.32), respectively, so that $\xi^0 = E' - B$ and $\xi = E$. The density perturbation $\delta\rho$ and the scalar velocity potential v are subject to the transformations (6.45) and (6.46), respectively, so we can construct the gauge-invariant variables:

$$\delta\rho^{(\text{GI})} = \delta\rho + \rho'(B - E'), \quad v^{(\text{GI})} = v + E'. \quad (7.18)$$

After the gauge-transformation to the Newtonian gauge ($\tilde{B} = 0 = \tilde{E}$), we have that $\tilde{\delta\rho}^{(\text{GI})} = \tilde{\delta\rho}$ and $\tilde{v}^{(\text{GI})} = \tilde{v}$. In the following, we omit the symbol “(GI)” and the tilde.

To characterize the trajectory of particles with mass m at a spacetime point $x^\mu = (\eta, x^i)$, we define the four momentum

$$P^\mu = \frac{dx^\mu}{d\lambda}, \quad (7.19)$$

where λ is the Affine parameter related to the proper time τ , as $\lambda = \tau/m$ for $m \neq 0$. Since the four velocity $u^\mu = dx^\mu/d\tau$ satisfies the relation $u^\mu u_\mu = -1$, the four momentum $P^\mu = mu^\mu$ obeys

$$g_{\mu\nu} P^\mu P^\nu + m^2 = 0. \quad (7.20)$$

For massless particles, we can choose the Affine parameter λ along the geodesic such that the four momentum is given by Eq. (7.19). In this case, the relation (7.20) is also valid by setting $m = 0$. Defining the momentum in the three-dimensional space as $p^2 = g_{ij} P^i P^j$, Eq. (7.20) translates to

$$-a^2(1 + 2\Psi)(P^0)^2 + E^2 = 0, \quad E^2 = p^2 + m^2, \quad (7.21)$$

where E is the energy of each particle. In what follows, we employ the linear approximation under which terms higher than first order in perturbations are neglected

relative to first-order terms. Then, Eq. (7.21) reduces to

$$P^0 = \frac{E}{a}(1 - \Psi). \quad (7.22)$$

The three-dimensional momentum P^i can be written as $P^i = Cn^i$, where C is a constant and n^i is a unit vector along P^i . Substituting this relation into $p^2 = g_{ij}P^iP^j$ and using $g_{ij} = a^2(1 + 2\Phi)\delta_{ij}$, we obtain $C = (p/a)(1 - \Phi)$ and hence

$$P^i = \frac{p}{a}(1 - \Phi)n^i. \quad (7.23)$$

To deal with the movement of particles statistically in the framework of GR, we consider a distribution function $f(x^\mu, P^\mu)$ that depends on the spacetime position x^μ and the four-momentum P^μ . Analogous to the fact that the spacetime volume element invariant under a coordinate transformation is $\sqrt{-g}d^4x$, the invariant volume element of four-momentum is given by $\sqrt{-g}d^4P$. Taking into account the fact that the particle is subject to the constraint (7.20), we define the invariant momentum element as

$$d\Pi = \frac{\sqrt{-g}d^4P}{(2\pi)^3}\theta(P^0)\delta(g_{\mu\nu}P^\mu P^\nu + m^2), \quad (7.24)$$

where $\delta(x)$ is the delta function, and $\theta(P^0)$ is the function satisfying $\theta(P^0) = 1$ for $P^0 > 0$ and $\theta(P^0) = 0$ for $P^0 < 0$. For the metric (7.17), we integrate Eq. (7.24) in the regime $P^0 > 0$. In this case we have $g_{\mu\nu}P^\mu P^\nu + m^2 = -[(bP^0)^2 - E^2]$, where $b = \sqrt{|g_{00}|} = a(1 + \Psi)$. On using the properties $\delta(x) = \delta(-x)$ and $\delta(x^2 - a^2) = [\delta(x - a) + \delta(x + a)]/(2a)$, Eq. (7.24) reduces to

$$d\Pi = \frac{\sqrt{-g}d^3P}{(2\pi)^3} \frac{1}{2E\sqrt{|g_{00}|}}. \quad (7.25)$$

Since $\sqrt{-g} = a^4(1 + \Psi + 3\Phi)$ and $d^3P = [(1 - 3\Phi)/a^3]d^3p$ from Eq. (7.23), we obtain

$$d\Pi = \frac{d^3p}{(2\pi)^3} \frac{1}{2E}. \quad (7.26)$$

For the distribution function f with g_* internal degrees of freedom, we define the energy-momentum tensor

$$T^\mu{}_\nu = 2g_* \int d\Pi P^\mu P_\nu f. \quad (7.27)$$

Since $d\Pi$ is given by Eq. (7.26), it follows that

$$T^\mu{}_\nu = \frac{g_*}{(2\pi)^3} \int d^3p \frac{P^\mu P_\nu}{E} f. \quad (7.28)$$

From Eqs. (7.22) and (7.23), we have $P_0 = -aE(1 + \Psi)$ and $P_i = ap(1 + \Phi)n_i$, where n_i is the unit vector defined by $n_i = \delta_{ij}n^j$. The distribution function f depends on η, x^i, P^0, P^i , among which P^0 and P^i depend on p and n^i through Eqs. (7.22)

and (7.23). Since the background part $f^{(0)}$ of the distribution function depends on p and η , we decompose f into the background and perturbed parts, as

$$f(\eta, x^i, p, n^i) = f^{(0)}(p, \eta) + \delta f(\eta, x^i, p, n^i). \quad (7.29)$$

Using the properties $\int d\Omega n^i = 0$ and $\int d\Omega n^i n_j = (4\pi/3)\delta^i_j$ for the integral with respect to the solid angle Ω , each component of T^μ_ν reduces to

$$T^0_0 = -\frac{g_*}{(2\pi)^3} \int d^3p E \left(f^{(0)} + \delta f \right), \quad (7.30)$$

$$T^0_i = \frac{g_*}{(2\pi)^3} \int d^3p p n_i \delta f, \quad (7.31)$$

$$T^i_j = \frac{g_*}{(2\pi)^3} \int d^3p \frac{p^2}{E} \left(\frac{1}{3} \delta^i_j f^{(0)} + n^i n_j \delta f \right). \quad (7.32)$$

As we derived in Eq. (6.40), the fluid energy–momentum tensor can be expressed as $T^0_0 = -(\rho + \delta\rho)$, $T^0_i = (\rho + P)v_{|i}$, and $T^i_j = (P + \delta P)\delta^i_j + \pi^i_j$, where ρ and P are the background density and the pressure with their perturbations $\delta\rho$ and δP respectively, v is the scalar velocity potential, and π^i_j is the anisotropic stress. Then, the background parts have the following correspondences

$$\rho = \frac{g_*}{(2\pi)^3} \int d^3p E f^{(0)}, \quad P = \frac{g_*}{(2\pi)^3} \int d^3p \frac{p^2}{3E} f^{(0)}, \quad (7.33)$$

which coincide with Eqs. (4.33) and (4.35), respectively. The perturbed parts are given by

$$\delta\rho = \frac{g_*}{(2\pi)^3} \int d^3p E \delta f, \quad (7.34)$$

$$v_{|i} = \frac{1}{\rho + P} \frac{g_*}{(2\pi)^3} \int d^3p p n_i \delta f, \quad (7.35)$$

$$\delta P = \frac{g_*}{(2\pi)^3} \int d^3p \frac{p^2}{3E} \delta f, \quad (7.36)$$

$$\pi^i_j = \frac{g_*}{(2\pi)^3} \int d^3p \frac{p^2}{E} \left(n^i n_j - \frac{1}{3} \delta^i_j \right) \delta f. \quad (7.37)$$

In Sec. 7.3, we will discuss how these macroscopic physical quantities are related to CMB temperature fluctuations.

To derive the equations of motion for matter perturbations of each species, we need to solve the Boltzmann equation

$$\frac{df}{d\lambda} = C[f], \quad (7.38)$$

where $C[f]$ is the collision term. Since f is a function of x^0 , x^i , p , n^i , the left hand side of Eq. (7.38) reads

$$\frac{df}{d\lambda} = P^0 \frac{\partial f}{\partial x^0} + P^i \frac{\partial f}{\partial x^i} + \frac{dp}{d\lambda} \frac{\partial f}{\partial p} + \frac{dn^i}{d\lambda} \frac{\partial f}{\partial n^i}, \quad (7.39)$$

where we used the four-momentum $P^\mu = dx^\mu/d\lambda$. The collision term $C[f]$ characterizes how much extent the particles move to another phase space through their interactions. In quantum field theory, it can be computed under the approximation that the collision occurs at short distances. If the scattering amplitude $\mathcal{M}$ of the interaction $X_1 + X_2 \leftrightarrow X_3 + X_4$ is the same for both left and right scatterings, the collision term associated with the particle with index 1 is given by

$$C[f(X_1)] = \frac{1}{2} \int d\Pi_2 \int d\Pi_3 \int d\Pi_4 (2\pi)^4 \delta^{(4)}(P_1 + P_2 - P_3 - P_4) |\mathcal{M}|^2 \\ \times [f_3 f_4 (1 \pm f_1)(1 \pm f_2) - f_1 f_2 (1 \pm f_3)(1 \pm f_4)], \quad (7.40)$$

where $d\Pi_i = d^3 p_i / [(2\pi)^3 2E_i]$ (with the particle energy E_i and the momentum p_i), and $\delta^{(4)}(P_1 + P_2 - P_3 - P_4) = \delta(E_1 + E_2 - E_3 - E_4) \delta^{(3)}(p_1 + p_2 - p_3 - p_4)$.

The plus and minus signs of the term $1 \pm f_i$ in Eq. (7.40) correspond to bosonic and fermionic particles, respectively. The production rate of the particle with index 1 is proportional to the product $f_3 f_4$, while the decreasing rate is in proportion to $f_1 f_2$. For fermions, the quantum state when a particle with index i is produced is proportional to $1 - f_i$. This corresponds to the Pauli exclusion principle, which states that, when a quantum state is occupied by a fermionic particle, the produced particle cannot enter the same state. For bosons, the proportionality factor is given by $1 + f_i$, so that the quantum state can be occupied by many particles.

Expanding the Boltzmann equation (7.38) up to first order in perturbations, we can obtain linearly perturbed equations of motion for each particle. In Sec. 7.3, we derive the perturbation equations of photons and in Sec. 7.4 we proceed to the discussion for baryons, dark matter and neutrinos.

7.3. Boltzmann equations for photons

Let us first discuss the case of photons (mass $m = 0$). Since $E = p$ in this case, we have $P^0 = (p/a)(1 - \Psi)$ from Eq. (7.22). At zeroth order in perturbations, the function f is independent of n^i , so the last term of Eq. (7.39) is second order in perturbations. The product of Φ and $\partial f / \partial x^i$ is also a second-order quantity. Up to linear order in perturbations, the left hand side of the Boltzmann equation reduces to

$$\frac{df}{d\lambda} = \frac{p}{a}(1 - \Psi) \frac{\partial f}{\partial \eta} + \frac{p}{a} n^i \frac{\partial f}{\partial x^i} + \frac{dp}{d\lambda} \frac{\partial f}{\partial p}. \quad (7.41)$$

In the following, we neglect all terms higher than first order. To obtain $dp/d\lambda$ in Eq. (7.41), we first derive the term $dp/d\eta$. In doing so, we use the fact that the temporal component P^0 of the four-momentum satisfies the geodesic equation $dP^0/d\lambda = -\Gamma_{\nu\lambda}^0 P^\nu P^\lambda$. Then, it follows that

$$\frac{1}{p} \frac{dp}{d\eta} = \mathcal{H} + \frac{d\Psi}{d\eta} - a^2 \Gamma_{\nu\lambda}^0 \frac{P^\nu P^\lambda}{p^2} (1 + 2\Psi), \quad (7.42)$$

where $\mathcal{H}$ is defined by Eq. (6.28). Since $dx^i/d\eta = P^i/P^0 = (1 + \Psi - \Phi)n^i$ from Eqs. (7.22) and (7.23), the η derivative of $\Psi(\eta, x^i(\eta))$ reads

$$\frac{d\Psi}{d\eta} = \frac{\partial\Psi}{\partial\eta} + \frac{dx^i}{d\eta} \frac{\partial\Psi}{\partial x^i} = \frac{\partial\Psi}{\partial\eta} + n^i \frac{\partial\Psi}{\partial x^i}. \quad (7.43)$$

The quantity $\Gamma_{\nu\lambda}^0 P^\nu P^\lambda/p^2$ is given by

$$\begin{aligned} \Gamma_{\nu\lambda}^0 \frac{P^\nu P^\lambda}{p^2} &= \frac{g^{00}}{2} \left(2 \frac{\partial g_{0\nu}}{\partial x^\lambda} - \frac{\partial g_{\nu\lambda}}{\partial\eta} \right) \frac{P^\nu P^\lambda}{p^2} \\ &= \frac{1 - 2\Psi}{a^2} \left(2\mathcal{H} + \frac{\partial\Psi}{\partial\eta} + \frac{\partial\Phi}{\partial\eta} + 2n^i \frac{\partial\Psi}{\partial x^i} \right). \end{aligned} \quad (7.44)$$

Substituting Eqs. (7.43) and (7.44) into Eq. (7.42), we obtain

$$\frac{1}{p} \frac{dp}{d\eta} = -\mathcal{H} - \frac{\partial\Phi}{\partial\eta} - n^i \frac{\partial\Psi}{\partial x^i}. \quad (7.45)$$

In the absence of perturbations we have that $(1/p)(dp/d\eta) = -\mathcal{H}$, so integration of this equation leads to the momentum dependence $p \propto 1/a$. Hence the physical wavelength is proportional to a . If there are the time and spatial variations of gravitational potentials, e.g., $\partial\Phi/\partial\eta$ and $\partial\Psi/\partial x^i$, the momentum p is also subject to modifications. Since $P^0 = d\eta/d\lambda = (p/a)(1 - \Psi)$, the quantity $dp/d\lambda$ in Eq. (7.41) reads $dp/d\lambda = (dp/d\eta)(p/a)(1 - \Psi)$. Hence Eq. (7.41) reduces to

$$\frac{df}{d\lambda} = \frac{p}{a} (1 - \Psi) \left[\frac{\partial f}{\partial\eta} - p \left(\mathcal{H} + \frac{\partial\Phi}{\partial\eta} + n^i \frac{\partial\Psi}{\partial x^i} \right) \frac{\partial f}{\partial p} \right] + \frac{p}{a} n^i \frac{\partial f}{\partial x^i}. \quad (7.46)$$

The distribution function of photons is given by

$$f = [\exp(p/T) - 1]^{-1}, \quad (7.47)$$

where the temperature T is a function of η at zeroth order, but the perturbation δT depends on η , x^i , n^i . Taking the partial derivatives of Eq. (7.47) with respect

to T and p , we obtain

$$\frac{\partial f}{\partial T} = -\frac{p}{T} \frac{\partial f}{\partial p}. \quad (7.48)$$

We define the function

$$\Theta(\eta, x^i, n^i) \equiv \frac{1}{4} \frac{\int dp p^3 \delta f(\eta, x^i, p, n^i)}{\int dp p^3 f^{(0)}(p)}, \quad (7.49)$$

which corresponds to temperature perturbations. Since $\delta f = -p(\partial f / \partial p) \delta T / T$ from Eq. (7.48), integrating Eq. (7.49) by parts and dropping the boundary term leads to the relation $\Theta = \delta T / T$. Substituting $f = f^{(0)} + \delta f$ into Eq. (7.46) and decomposing $df/d\lambda$ in terms of zeroth and first-order contributions, it follows that

$$\begin{aligned} \frac{df}{d\lambda} = & \frac{p}{a} \left(\frac{\partial f^{(0)}}{\partial \eta} - p\mathcal{H} \frac{\partial f^{(0)}}{\partial p} \right) \\ & + \frac{p}{a} \left[\frac{\partial \delta f}{\partial \eta} + n^i \frac{\partial \delta f}{\partial x^i} - p\mathcal{H} \frac{\partial \delta f}{\partial p} - p \frac{\partial f^{(0)}}{\partial p} \left(\frac{\partial \Phi}{\partial \eta} + n^i \frac{\partial \Psi}{\partial x^i} \right) \right] \\ & - \frac{p}{a} \Psi \left(\frac{\partial f^{(0)}}{\partial \eta} - p\mathcal{H} \frac{\partial f^{(0)}}{\partial p} \right). \end{aligned} \quad (7.50)$$

The first line on the right hand side of Eq. (7.50) reduces to

$$\frac{df^{(0)}}{d\lambda} = -\frac{p^2}{a} \frac{\partial f^{(0)}}{\partial p} \left(\frac{1}{T} \frac{\partial T}{\partial \eta} + \mathcal{H} \right). \quad (7.51)$$

Using the fact that the photon temperature decreases as $T \propto a^{-1}$ at zeroth order, we obtain $df^{(0)}/d\lambda = 0$. As we will see later, this is attributed to the fact that the collision term on the right hand side of the Boltzmann equation vanishes at zeroth order. Substituting the relation $\delta f = -p(\partial f^{(0)}/\partial p)\Theta$ into Eq. (7.50), the perturbed part reduces to

$$\frac{d}{d\lambda} \delta f = -\frac{p^2}{a} \frac{\partial f^{(0)}}{\partial p} \left(\frac{\partial \Theta}{\partial \eta} + n^i \frac{\partial \Theta}{\partial x^i} + \frac{\partial \Phi}{\partial \eta} + n^i \frac{\partial \Psi}{\partial x^i} \right). \quad (7.52)$$

The next step is the derivation of the collision term $C_\gamma[f]$ for the Thomson scattering: $\gamma(\mathbf{p}) + e^-(\mathbf{q}) \leftrightarrow \gamma(\mathbf{p}') + e^-(\mathbf{q}')$, where we explicitly wrote down the momenta of photons and electrons before and after the scattering. If the rest energy of electrons (m_e) is much smaller than the photon temperature T , the electron distribution function f_e is much smaller than 1, so we can approximate $1 - f_e(\mathbf{q}) \simeq 1$. For the photon distribution function f , the collision term of Thomson scattering is given by

$$\begin{aligned} C_\gamma[f(\mathbf{p})] = & \frac{1}{2} \int d\Pi_q \int d\Pi_{p'} \int d\Pi_{q'} (2\pi)^4 \delta^{(4)}(P + Q - P' - Q') |\mathcal{M}|^2 \\ & \times \left\{ f(\mathbf{p}') f_e(\mathbf{q}') [1 + f(\mathbf{p})] - f(\mathbf{p}) f_e(\mathbf{q}) [1 + f(\mathbf{p}')] \right\}, \end{aligned} \quad (7.53)$$

where $\delta^{(4)}(P + Q - P' - Q') = \delta(p^0 + q^0 - p'^0 - q'^0)\delta^{(3)}(\mathbf{p} + \mathbf{q} - \mathbf{p}' - \mathbf{q}')$. The photon energy is given by $E_\gamma = p^0 = p$, so that $d\Pi_{p'} = d^3p'/[(2\pi)^3 2p']$. Since we are considering non-relativistic electrons, it follows that $d\Pi_q = d^3q/[(2\pi)^3 2m_e]$ and $d\Pi_{q'} = d^3q'/[(2\pi)^3 2m_e]$. The calculation based on the interaction of quantum fields leads to the scattering amplitude $\mathcal{M}$, as [6, 7]

$$|\mathcal{M}|^2 = 24\pi m_e^2 \sigma_T (1 + \cos^2 \theta), \quad (7.54)$$

where θ is the angle between the momenta $\mathbf{p}$ and $\mathbf{p}'$ before and after the scattering, respectively, and $\sigma_T = 8\pi\alpha^2/(3m_e^2) = 6.65 \times 10^{-29} \text{ m}^2$ is the total cross-section ($\alpha = 1/137$ is the fine-structure constant). Denoting the unit vectors along the directions of $\mathbf{p}$ and $\mathbf{p}'$ as $\mathbf{n}$ and $\mathbf{n}'$ respectively, it follows that $\cos\theta = \mathbf{n} \cdot \mathbf{n}'$. Since the kinetic energy of non-relativistic electrons is approximately given by $E_e(q) = q^0 = m_e + q^2/(2m_e)$, the temporal part of the delta function in Eq. (7.53) reduces to $\delta(p - p' + (q^2 - q'^2)/(2m_e))$. Hence Eq. (7.53) yields

$$\begin{aligned} C_\gamma[f(\mathbf{p})] &= \frac{3\sigma_T}{64\pi^4} \int d^3q \int d^3q' \int d^3p' \frac{1}{p'} [1 + (\mathbf{n} \cdot \mathbf{n}')^2] \\ &\quad \times \delta(p - p' + (q^2 - q'^2)/(2m_e)) \delta^{(3)}(\mathbf{p} + \mathbf{q} - \mathbf{p}' - \mathbf{q}') \\ &\quad \times \{f(\mathbf{p}')f_e(\mathbf{q}')[1 + f(\mathbf{p})] - f(\mathbf{p})f_e(\mathbf{q})[1 + f(\mathbf{p}')]\}. \end{aligned} \quad (7.55)$$

To perform the integral in terms of q' in Eq. (7.55), we employ the relation $\mathbf{q}' = \mathbf{q} + \mathbf{p} - \mathbf{p}'$. For the Thomson scattering the electron momentum $|\mathbf{q}|$ is much smaller than $|\mathbf{p} - \mathbf{p}'|$, so we have the approximate relation

$$\delta(p - p' + (q^2 - q'^2)/(2m_e)) \simeq \delta(p - p') + \frac{\mathbf{q} \cdot (\mathbf{p} - \mathbf{p}')}{m_e} \frac{\partial}{\partial p'} \delta(p - p'), \quad (7.56)$$

which was expanded around $\delta(p - p')$. The electron distribution function is given by $f_e(\mathbf{q}') = f_e(\mathbf{q} + \mathbf{p} - \mathbf{p}') \simeq f_e(\mathbf{q}) + (\partial f_e / \partial \mathbf{q}) \cdot (\mathbf{p} - \mathbf{p}')$, so the terms on the third line of Eq. (7.55) reduce to

$$f_e(\mathbf{q})[f(\mathbf{p}') - f(\mathbf{p})] + \frac{\partial f_e}{\partial \mathbf{q}} \cdot (\mathbf{p} - \mathbf{p}') f(\mathbf{p}') [1 + f(\mathbf{p})]. \quad (7.57)$$

Since the second term corresponds to a boundary term, Eq. (7.55) reduces to

$$\begin{aligned} C_\gamma[f(\mathbf{p})] &= \frac{3\sigma_T}{64\pi^4} \int d^3q f_e(\mathbf{q}) \int d^3p' \frac{1}{p'} [1 + (\mathbf{n} \cdot \mathbf{n}')^2] [f(\mathbf{p}') - f(\mathbf{p})] \\ &\quad \times \left[\delta(p - p') + \frac{\mathbf{q} \cdot (\mathbf{p} - \mathbf{p}')}{m_e} \frac{\partial}{\partial p'} \delta(p - p') \right]. \end{aligned} \quad (7.58)$$

We employ the fact that the electron number density n_e and the velocity $\mathbf{v}_b$ are given, respectively, by

$$n_e = 2 \int \frac{d^3q}{(2\pi)^3} f_e(\mathbf{q}), \quad \mathbf{v}_b = \frac{2}{n_e} \int \frac{d^3q}{(2\pi)^3} \frac{\mathbf{q}}{m_e} f_e(\mathbf{q}). \quad (7.59)$$

Then, Eq. (7.58) can be expressed as

$$C_\gamma[f(\mathbf{p})] = \frac{3\sigma_T n_e}{16\pi} \int d^3p' \frac{1}{p'} [1 + (\mathbf{n} \cdot \mathbf{n}')^2] [f(\mathbf{p}') - f(\mathbf{p})] \\ \times \left[\delta(p - p') + \mathbf{v}_b \cdot (\mathbf{p} - \mathbf{p}') \frac{\partial}{\partial p'} \delta(p - p') \right]. \quad (7.60)$$

Substituting the relations $f(\mathbf{p}) = f^{(0)}(p) + \delta f(p, \mathbf{n})$ and $f(\mathbf{p}') = f^{(0)}(p') + \delta f(p', \mathbf{n}')$ into Eq. (7.60) and rewriting the integral of p' with respect to Ω' , it follows that

$$C_\gamma[f(\mathbf{p})] = \frac{3\sigma_T n_e}{16\pi} \int dp' p' \int d\Omega' [1 + (\mathbf{n} \cdot \mathbf{n}')^2] \left[(\delta f(p', \mathbf{n}') - \delta f(p, \mathbf{n})) \right. \\ \left. \times \delta(p - p') + (f^{(0)}(p') - f^{(0)}(p)) \mathbf{v}_b \cdot (\mathbf{p} - \mathbf{p}') \frac{\partial \delta(p - p')}{\partial p'} \right] \\ = \frac{3\sigma_T n_e}{16\pi} p \int d\Omega' [1 + (\mathbf{n} \cdot \mathbf{n}')^2] \left[\delta f(p, \mathbf{n}') - \delta f(p, \mathbf{n}) - \frac{\partial f^{(0)}}{\partial p} \mathbf{v}_b \cdot \mathbf{p} \right]. \quad (7.61)$$

The collision term vanishes at zeroth order of perturbations. Plugging the relation $\delta f(p, \mathbf{n}) = -p(\partial f^{(0)}/\partial p)\Theta$ into Eq. (7.61) and using $\mathbf{n} = \mathbf{p}/p$, we finally obtain

$$C_\gamma[f(\mathbf{p})] = -\frac{3\sigma_T n_e}{16\pi} p^2 \frac{\partial f^{(0)}}{\partial p} \int d\Omega' [1 + (\mathbf{n} \cdot \mathbf{n}')^2] [\Theta(\mathbf{n}') - \Theta(\mathbf{n}) + \mathbf{n} \cdot \mathbf{v}_b]. \quad (7.62)$$

From Eqs. (7.52) and (7.62), the perturbed Boltzmann equation of photons is

$$\frac{\partial \Theta}{\partial \eta} + n^i \frac{\partial \Theta}{\partial x^i} + \frac{\partial \Phi}{\partial \eta} + n^i \frac{\partial \Psi}{\partial x^i} \\ = \frac{3\sigma_T n_e a}{16\pi} \int d\Omega' [1 + (\mathbf{n} \cdot \mathbf{n}')^2] [\Theta(\mathbf{n}') - \Theta(\mathbf{n}) + \mathbf{n} \cdot \mathbf{v}_b]. \quad (7.63)$$

We expand the perturbed quantities Θ , Φ , Ψ in terms of Fourier series, as

$$\Theta = \frac{1}{(2\pi)^3} \int d^3k \Theta_k e^{i\mathbf{k} \cdot \mathbf{x}}, \quad (7.64)$$

where $\mathbf{k} \cdot \mathbf{x} = k_i x^i$. The scalar velocity potential v_b , which is related to $\mathbf{v}_b$ as $\mathbf{v}_b = \partial v_b / \partial x^i$, is also expanded in Fourier series. Defining the quantity

$$\mu = \frac{\mathbf{n} \cdot \mathbf{k}}{k} = \frac{n^i k_i}{k}, \quad (7.65)$$

the Fourier mode of Eq. (7.63) with the comoving wavenumber k obeys

$$\Theta' + i\mu k \Theta + \Phi' + i\mu k \Psi \\ = \frac{3\sigma_T n_e a}{16\pi} \int d\Omega' [1 + (\mathbf{n} \cdot \mathbf{n}')^2] [\Theta(\mathbf{n}') - \Theta(\mathbf{n}) + i\mu k v_b], \quad (7.66)$$

where a prime represents a partial derivative with respect to η , and we omitted the subscript k .

Using the spherical harmonics Y_l^m , we expand the temperature perturbation Θ in the form

$$\Theta(\mathbf{n}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l a_{lm} Y_l^m(\mathbf{n}), \quad (7.67)$$

where $Y_l^m(\mathbf{n})$ satisfies the orthogonal relation

$$\int d\Omega Y_l^{m*}(\mathbf{n}) Y_{l'}^{m'}(\mathbf{n}) = \delta_{ll'} \delta_{mm'}. \quad (7.68)$$

The Legendre polynomial defined by

$$\mathcal{P}_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l \quad (7.69)$$

is related to Y_l^m , as

$$\mathcal{P}_l(\mathbf{n} \cdot \mathbf{n}') = \frac{4\pi}{2l+1} \sum_m Y_l^m(\mathbf{n}) Y_l^{m*}(\mathbf{n}'). \quad (7.70)$$

Since $\mathcal{P}_0(\mu) = 1$, $\mathcal{P}_1(\mu) = \mu$, $\mathcal{P}_2(\mu) = (3\mu^2 - 1)/2$ from Eq. (7.69), the term $1 + (\mathbf{n} \cdot \mathbf{n}')^2$ in Eq. (7.63) is equivalent to $(4/3)\mathcal{P}_0(\mathbf{n} \cdot \mathbf{n}') + (2/3)\mathcal{P}_2(\mathbf{n} \cdot \mathbf{n}')$. Substituting Eq. (7.70) into this relation and using Eqs. (7.67) and (7.68), we can compute the term $\int d\Omega' [1 + (\mathbf{n} \cdot \mathbf{n}')^2] \Theta(\mathbf{n}')$. The contributions $\int d\Omega' [1 + (\mathbf{n} \cdot \mathbf{n}')^2] [-\Theta(\mathbf{n}) + i\mu k v_b]$ reduce to $(16\pi/3)[- \Theta(\mathbf{n}) + i\mu k v_b]$ by using the relations $\mathbf{n} \cdot \mathbf{n}' = \cos \theta$ and $d\Omega' = 2\pi \sin \theta d\theta$. In summary, Eq. (7.66) can be expressed as

$$\begin{aligned} & \Theta' + i\mu k \Theta + \Phi' + i\mu k \Psi \\ &= \sigma_T n_e a \left[a_{00} Y_0^0(\mathbf{n}) + \frac{1}{10} \sum_m a_{2m} Y_2^m(\mathbf{n}) - \Theta(\mathbf{n}) + i\mu k v_b \right]. \end{aligned} \quad (7.71)$$

We define the quantity Θ_l according to the relation

$$a_{lm} = 4\pi (-i)^l \Theta_l Y_l^{m*}(\hat{\mathbf{k}}), \quad (7.72)$$

where $\hat{\mathbf{k}} = \mathbf{k}/k$. On using the relation (7.70), we obtain

$$\sum_m a_{lm} Y_l^m(\mathbf{n}) = (-i)^l (2l+1) \Theta_l \mathcal{P}_l(\mu), \quad (7.73)$$

so Eq. (7.67) can be expressed as

$$\Theta = \sum_{l=0}^{\infty} (-i)^l (2l+1) \Theta_l(k, \eta) \mathcal{P}_l(\mu). \quad (7.74)$$

Hence the dependence of Θ on $\mathbf{n}$ appears inside of $\mathcal{P}_l(\mu)$ as a function of μ . From Eq. (7.73), we have that $a_{00} Y_0^0 = \Theta_0$ and $\sum_m a_{2m} Y_2^m(\mathbf{n}) = -5\Theta_2 \mathcal{P}_2(\mu)$,

so Eq. (7.71) reduces to

$$\Theta' + i\mu k\Theta + \Phi' + i\mu k\Psi = \sigma_T n_e a \left[\Theta_0 - \Theta + i\mu k v_b - \frac{1}{2} \mathcal{P}_2(\mu) \Theta_2 \right]. \quad (7.75)$$

Multiplying Eq. (7.74) by $\mathcal{P}_{l'}(\mu)$ and integrating it with respect to μ from -1 to 1 , and using the orthogonal relation

$$\int_{-1}^{+1} \frac{d\mu}{2} \mathcal{P}_l(\mu) \mathcal{P}_{l'}(\mu) = \frac{1}{2l+1} \delta_{ll'}, \quad (7.76)$$

it follows that

$$\Theta_l(k, \eta) = i^l \int_{-1}^{+1} \frac{d\mu}{2} \Theta \mathcal{P}_l(\mu). \quad (7.77)$$

Multiplying Eq. (7.75) by $\mathcal{P}_l(\mu)$ ($l = 0, 1, 2, \dots$) and employing the orthogonal relation (7.76) as well as the recurrence relation

$$(l+1)\mathcal{P}_{l+1}(\mu) = (2l+1)\mu\mathcal{P}_l(\mu) - l\mathcal{P}_{l-1}(\mu), \quad (7.78)$$

we obtain the following system of differential equations with respect to Θ_l of the multipole expansion:

$$\Theta'_0 + k\Theta_1 + \Phi' = 0, \quad (7.79)$$

$$\Theta'_1 - \frac{k}{3}(\Theta_0 + \Psi - 2\Theta_2) = -\sigma_T n_e a \left(\Theta_1 + \frac{1}{3} k v_b \right), \quad (7.80)$$

$$\Theta'_2 + \frac{k}{5}(3\Theta_3 - 2\Theta_1) = -\frac{9}{10} \sigma_T n_e a \Theta_2, \quad (7.81)$$

$$\Theta'_l + \frac{k}{2l+1} [(l+1)\Theta_{l+1} - l\Theta_{l-1}] = -\sigma_T n_e a \Theta_l \quad (l \geq 3). \quad (7.82)$$

These equations are not closed, but the dominant contributions to perturbations relevant to CMB temperature anisotropies correspond to the modes with low multipoles. To confirm this property, we define the optical depth characterizing the interaction strength between photons and baryons as

$$\tau = \int_{\eta}^{\eta_0} d\tilde{\eta} n_e(\tilde{\eta}) a(\tilde{\eta}) \sigma_T, \quad (7.83)$$

where η_0 is the present value of η . Before the CMB decoupling epoch, τ is much larger than 1. As n_e decreases, τ gets smaller. The right hand side of Eq. (7.82) can be estimated as $\tau' \Theta_l \approx \tau \Theta_l / \eta \approx \tau a H \Theta_l$. The first term on the left hand side of Eq. (7.82) is of the order of Θ/η , so it can be neglected relative to the right hand side

of it in the regime $\tau \gg 1$. From the balance between the right hand side of Eq. (7.82) and the third term on the left hand side of it, we obtain

$$\Theta_l \approx \frac{1}{\tau} \frac{k}{aH} \Theta_{l-1}. \quad (7.84)$$

For perturbations with the wavelength of the order of the Hubble radius ($k \sim aH$), we have that $\Theta_l \ll \Theta_{l-1}$ for $\tau \gg 1$. In this case, the second term on the left hand side of Eq. (7.82) can be neglected relative to the third term. In the strong coupling regime of photons, the perturbations Θ_l with low l give the dominant contribution.

Let us discuss how the terms Θ_0 , Θ_1 , Θ_2 are related to macroscopic physical quantities. We substitute Eq. (7.49) into Eq. (7.77) and use the fact that the background photon density ρ_γ is given by $\rho_\gamma = \frac{g_*}{2\pi^2} \int dp p^3 f^{(0)}(p)$ from Eq. (7.33). Then, we obtain

$$\Theta_l = \frac{i^l g_*}{16\pi^2 \rho_\gamma} \int_{-1}^{+1} d\mu \int dp p^3 \mathcal{P}_l(\mu) \delta f = \frac{i^l g_*}{4\rho_\gamma} \int \frac{d^3 p}{(2\pi)^3} p \mathcal{P}_l(\mu) \delta f. \quad (7.85)$$

From Eq. (7.34), the perturbation of the photon energy density is given by $\delta\rho_\gamma = \frac{g_*}{(2\pi)^3} \int d^3 p p \delta f$, and hence

$$\Theta_0 = \frac{1}{4} \delta\gamma, \quad \delta\gamma = \frac{\delta\rho_\gamma}{\rho_\gamma}. \quad (7.86)$$

For the Fourier mode v_γ of the photon velocity potential, Eq. (7.35) gives

$$v_\gamma = -\frac{i}{k} \frac{3}{4\rho_\gamma} g_* \int \frac{d^3 p}{(2\pi)^3} p \mu \delta f, \quad (7.87)$$

so this quantity is related to Θ_1 , as

$$\Theta_1 = -\frac{1}{3} k v_\gamma. \quad (7.88)$$

According to Eq. (6.41), the anisotropic stress π^i_j of Eq. (7.37) has the relation with the scalar quantity Π_γ , as $\pi^i_j = \Pi_\gamma \delta^i_j - (1/3) \nabla^2 \Pi_\gamma$. The corresponding Fourier mode can be expressed as

$$\Pi_\gamma = -\frac{3}{2k^4} g_* \int \frac{d^3 p}{(2\pi)^3} p \left[(\mathbf{k} \cdot \mathbf{n})^2 - \frac{1}{3} k^2 \right]. \quad (7.89)$$

Comparing this with the quantity Θ_2 , we have the correspondence

$$\Theta_2 = \frac{k^2 \Pi_\gamma}{4\rho_\gamma}. \quad (7.90)$$

In summary, the perturbations Θ_0 , Θ_1 , Θ_2 correspond to the photon density perturbation, the velocity potential, and the anisotropic stress, respectively. Substituting Eqs. (7.86), (7.88) and (7.90) into Eqs. (7.79) and (7.80), we obtain

$$\delta'_\gamma - \frac{4}{3}k^2 v_\gamma + 4\Phi' = 0, \quad (7.91)$$

$$v'_\gamma + \frac{1}{4}\delta_\gamma + \Psi - \frac{k^2 \Pi_\gamma}{2\rho_\gamma} = \sigma_T n_e a(v_b - v_\gamma), \quad (7.92)$$

respectively.

We need the information of baryon perturbations to solve the differential equations (7.79)–(7.82). Moreover, the perturbations of dark matter affect the evolution of gravitational potentials, so we also require the equations of motion of dark matter. Besides photons, there exists the perturbation of neutrinos. In Sec. 7.4, we will derive the equations of motion for baryons, dark matter, and neutrinos.

7.4. Perturbation equations of baryons, dark matter, and neutrinos

Before the CMB decoupling the baryon fluid (composed of electrons and protons) was scattered by photons, so they behaved as a single photon–baryon fluid. The baryon fluid exchanges the energy and momentum through the Thomson scattering with photons, so the sum of energy–momentum tensors of baryons and photons is conserved. To derive the equations of motion for baryon perturbations, we use the fact that covariant derivatives of the perturbed energy–momentum tensor with respect to $\nu = 0$ and $\nu = i$ are given, respectively, by Eqs. (6.104) and (6.106).

For photons the pressure is given by $P_\gamma = \rho_\gamma/3$ at zeroth order in perturbations, so the energy density ρ_γ obeys the continuity equation $\dot{\rho}_\gamma + 4H\rho_\gamma = 0$. Moreover, the perturbed quantity defined by Eq. (6.49) reads $\delta q_\gamma = (4/3)a\rho_\gamma v_\gamma$ for the line element (7.17). In Fourier space, the covariant derivatives (6.104) and (6.106) associated with the perturbations of photons reduce, respectively, to

$${}^{(\gamma)}\delta T^\mu{}_{0;\mu} = -\rho_\gamma \left(\delta'_\gamma - \frac{4}{3}k^2 v_\gamma + 4\Phi' \right) = 0, \quad (7.93)$$

$${}^{(\gamma)}\delta T^\mu{}_{i;\mu} = \frac{4}{3}\rho_\gamma \left(v'_\gamma + \frac{1}{4}\delta_\gamma + \Psi - \frac{k^2 \Pi_\gamma}{2\rho_\gamma} \right) \Big|_i = \frac{4}{3}\rho_\gamma \sigma_T n_e a(v_b - v_\gamma)|_i, \quad (7.94)$$

where we used Eqs. (7.91) and (7.92). For $v_b \neq v_\gamma$, the perturbation ${}^{(\gamma)}\delta T^\mu{}_{i;\mu}$ does not vanish.

For baryons, we can employ the approximation that, after the electron becomes non-relativistic (the photon temperature below 0.511 MeV), the pressure and the anisotropic stress of baryons vanish. Then, the covariant derivatives (6.104) and

(6.106) for baryon density perturbations $\delta\rho_b$ reduce, respectively, to

$${}^{(b)}\delta T^\mu_{0;\mu} = -\rho_b (\delta'_b - k^2 v_b + 3\Phi'), \quad (7.95)$$

$${}^{(b)}\delta T^\mu_{i;\mu} = \rho_b (v'_b + \mathcal{H}v_b + \Psi)|_i, \quad (7.96)$$

where $\delta_b = \delta\rho_b/\rho_b$. On using the conservation law ${}^{(\gamma)}\delta T^\mu_{\nu;\mu} = -{}^{(b)}\delta T^\mu_{\nu;\mu}$ between photons and baryons, we obtain the equation of motion for baryon perturbations:

$$\delta'_b - k^2 v_b + 3\Phi' = 0, \quad (7.97)$$

$$v'_b + \mathcal{H}v_b + \Psi = -\frac{4\rho_\gamma}{3\rho_b}\sigma_T n_e a (v_b - v_\gamma). \quad (7.98)$$

The CDM can be regarded as non-relativistic matter with gravitational interactions alone, so that the collision term in the Boltzmann equation vanishes. Changing the subscript “ b ” of Eqs. (7.95) and (7.96) to “ c ” and using ${}^{(c)}\delta T^\mu_{\nu;\mu} = 0$, the density perturbation $\delta_c = \delta\rho_c/\rho_c$ and the velocity potential v_c of CDM obey

$$\delta'_c - k^2 v_c + 3\Phi' = 0, \quad (7.99)$$

$$v'_c + \mathcal{H}v_c + \Psi = 0, \quad (7.100)$$

respectively.

For neutrinos, we consider the nearly massless case in which they have behaved as relativistic particles by today. After the neutrino decoupling, we can deal with them as collisionless particles. We decompose the neutrino distribution function $f_\nu = [\exp(p/T) + 1]^{-1}$ into the background and perturbed parts, as $f_\nu = f_\nu^{(0)}(p) + \delta f_\nu(\eta, x^i, p, n^i)$. We define the quantity

$$\bar{\mathcal{N}} \equiv \frac{1}{4} \frac{\int dp p^3 \delta f_\nu(\eta, x^i, p, n^i)}{\int dp p^3 f_\nu^{(0)}(p)}, \quad (7.101)$$

which is analogous to the photon temperature perturbation (7.49). Taking note that the relation (7.48) holds for neutrinos as well, the left hand side of the Boltzmann equation is the same as that for photons. The perturbed equation for neutrinos can be derived by changing Θ to $\bar{\mathcal{N}}$ and setting the right hand side of Eq. (7.75) to be 0, i.e.,

$$\bar{\mathcal{N}}' + i\mu k \bar{\mathcal{N}} + \Phi' + i\mu k \Psi = 0. \quad (7.102)$$

We expand the function $\bar{\mathcal{N}}$ in terms of the Legendre polynomials as

$$\bar{\mathcal{N}} = \sum_{l=0}^{\infty} (-i)^l (2l+1) \mathcal{N}_l(k, \eta) \mathcal{P}_l(\mu). \quad (7.103)$$

In Fourier space, the multipoles $\mathcal{N}_l$ obey the differential equations

$$\mathcal{N}'_0 + k\mathcal{N}_1 + \Phi' = 0, \quad (7.104)$$

$$\mathcal{N}'_1 - \frac{k}{3}(\mathcal{N}_0 + \Psi - 2\mathcal{N}_2) = 0, \quad (7.105)$$

$$\mathcal{N}'_l + \frac{k}{2l+1}[(l+1)\mathcal{N}_{l+1} - l\mathcal{N}_{l-1}] = 0 \quad (l \geq 2). \quad (7.106)$$

There are the following correspondences $\mathcal{N}_0 = \delta\rho_\nu/(4\rho_\nu)$, $\mathcal{N}_1 = -kv_\nu/3$, and $\mathcal{N}_2 = k^2\Pi_\nu/(4\rho_\nu)$, where $\delta\rho_\nu$, v_ν , and Π_ν are the density perturbation, the velocity potential, and the anisotropic stress of neutrinos, respectively.

Dark energy does not usually cluster due to its negative pressure, so we neglect the dark energy perturbation in the following discussion.

In Sec. 6, we already derived the perturbed Einstein equations (6.97), (6.98), (6.100) and (6.101) in the presence of a fluid, so we just need to take into account all matter species for the perturbations $\delta\rho$, δq , Π , and δP . Then, the perturbed Einstein equations yield

$$3\mathcal{H}(\Phi' - \mathcal{H}\Psi) + k^2\Phi = 4\pi Ga^2(\rho_m\delta_m + 4\rho_r\Theta_{r,0}), \quad (7.107)$$

$$\Phi' - \mathcal{H}\Psi = 4\pi Ga^2(\rho_mv_m - 4\rho_r\Theta_{r,1}/k), \quad (7.108)$$

$$k^2(\Psi + \Phi) = -32\pi Ga^2\rho_r\Theta_{r,2}, \quad (7.109)$$

$$\Phi'' + \mathcal{H}(2\Phi' - \Psi') - (\mathcal{H}^2 + 2\mathcal{H}')\Psi = -\frac{16}{3}\pi Ga^2(\rho_r\Theta_{r,0} - 2\rho_r\Theta_{r,2}). \quad (7.110)$$

The subscript “ m ” represents the contributions from CDM and baryons, i.e.,

$$\rho_m\delta_m \equiv \rho_c\delta_c + \rho_b\delta_b, \quad (7.111)$$

$$\rho_mv_m \equiv \rho_cv_c + \rho_bv_b, \quad (7.112)$$

whereas the subscript “ r ” corresponds to the contributions from photons and neutrinos:

$$\rho_r\Theta_{r,i} \equiv \rho_\gamma\Theta_i + \rho_\nu\mathcal{N}_i, \quad (7.113)$$

where $i = 0, 1, 2$.

While we have focused on scalar perturbations in the above discussion, there exists the primordial tensor perturbation generated during inflation (whose amplitude is suppressed relative to that of the scalar perturbation). The tensor perturbation obeys Eq. (6.112) in the Universe dominated by a perfect fluid.

7.5. Initial conditions for perturbations

During inflation, the quantum fluctuations were stretched over the super-Hubble scales due to the rapid cosmic acceleration. The amplitude of the curvature perturbation $\mathcal{R}$ is frozen from the first Hubble radius exit during inflation to the second Hubble radius re-entry after inflation. For the perturbations with larger wavelengths, the second Hubble radius crossing occurs later. The largest scale observed in CMB measurements corresponds to $H_0^{-1} \approx 10^{28}$ cm. The perturbation whose wavelength is of the order of 10^{28} cm is re-entering the Hubble radius today.

Right after the end of inflation, the wavelength of observed CMB anisotropies ($2 \leq l \lesssim 1000$) is much larger than the Hubble radius at that time. To derive the initial conditions of perturbations during the radiation era, we discuss the evolution of super-Hubble perturbations characterized by $k \ll \mathcal{H} = aH$. Dropping the terms containing k in Eqs. (7.97), (7.99), (7.79), (7.104) and (7.107), and neglecting the contribution of non-relativistic matter on the right hand side of Eq. (7.107), it follows that

$$\delta'_b = -3\Phi', \quad \delta'_c = -3\Phi', \quad (7.114)$$

$$\Theta'_0 = -\Phi', \quad \mathcal{N}'_0 = -\Phi', \quad (7.115)$$

$$3\mathcal{H}(\Phi' - \mathcal{H}\Psi) = 4\pi G a^2 (4\rho_\gamma \Theta_0 + 4\rho_\nu \mathcal{N}_0). \quad (7.116)$$

From Eqs. (7.114) and (7.115), we have that $\delta'_b = \delta'_c = 3\Theta'_0 = 3\mathcal{N}'_0$. Integrating these equations with respect to η and setting the integration constant 0, we obtain

$$\delta_b = \delta_c = 3\Theta_0 = 3\mathcal{N}_0. \quad (7.117)$$

This is known as adiabatic initial conditions, in which case $\delta_m = \delta\rho_m/\rho_m = 3\delta T/T$ and $\Theta_0 = \delta\rho_r/(4\rho_r) = \delta T/T$. Non-adiabatic perturbations satisfying the initial condition $\delta\rho_r = -\delta\rho_m$ are called isocurvature perturbations. The observed perturbations in CMB and large-scale structure measurements are consistent with adiabatic initial conditions (7.117).

Using the adiabatic solution (7.117) and the Friedmann equation $3\mathcal{H}^2 = 8\pi G a^2 (\rho_\gamma + \rho_\nu)$ in the radiation era, Eq. (7.116) reduces to

$$\Phi' - \mathcal{H}\Psi = 2\mathcal{H}\Theta_0. \quad (7.118)$$

Neglecting the anisotropic stress of radiation in Eq. (7.109), it follows that $\Psi = -\Phi$. On using this relation and Eq. (7.115), differentiation of Eq. (7.118) with respect to η gives

$$\Phi'' + \left(3\mathcal{H} - \frac{\mathcal{H}'}{\mathcal{H}}\right)\Phi' = 0. \quad (7.119)$$

Since $a \propto \eta$ and $\mathcal{H} = 1/\eta$ during the radiation domination, the solution to Eq. (7.119) can be expressed as $\Phi = C_1 + C_2/\eta^3$, where C_1 and C_2 are integration constants. Neglecting the decaying mode, we have that $\Phi = C_1 = \text{constant}$ and

hence $\Psi = -2\Theta_0$ from Eq. (7.118). Then, the adiabatic initial conditions at $\eta = 0$ are given by

$$\Psi(0) = -\Phi(0) = -2\Theta_0(0), \quad (7.120)$$

$$\delta_b(0) = \delta_c(0) = 3\Theta_0(0) = 3\mathcal{N}_0(0). \quad (7.121)$$

Equations (7.114) and (7.115) are valid for super-Hubble perturbations ($k \ll \mathcal{H}$) during the matter era. Integrating the first of Eq. (7.115) with respect to η , we obtain the solution $\Theta_0 = -\Phi + C$. From Eq. (7.120), the integration constant C is fixed as $3\Phi(0)/2$, so that

$$\Theta_0(\eta) = -\Phi(\eta) + \frac{3}{2}\Phi(0). \quad (7.122)$$

To study the evolution of Θ_0 after the radiation era, we need to know how Φ varies during the transient period from the radiation era to the matter era. We will discuss this issue in Sec. 7.6.

Let us next derive the initial condition of velocity potentials. Around the early stage of the radiation era, photons are strongly coupled to baryons, so their velocity potentials v_γ and v_b are equivalent to each other. In this case we have $\Theta_1 = -kv_\gamma/3 = -kv_b/3$, so the photon equation (7.80) is of the same form as the neutrino equation (7.105). Moreover, the baryon equation (7.98) has the same form as the CDM equation (7.100). Using the solution $\Psi = \text{constant}$ and solving Eq. (7.100) under the initial condition $v_c = 0$, it follows that $v_c = -\Psi/(2\mathcal{H})$. In summary, the initial conditions of velocity potentials v_b and v_c are given by

$$\Theta_1(0) = \mathcal{N}_1(0) = -\frac{1}{3}kv_b = -\frac{1}{3}kv_c = \frac{k}{6\mathcal{H}}\Psi. \quad (7.123)$$

In the above discussion we have neglected the radiation anisotropic stress, but we will estimate its effect in the following. In the limit that $k \rightarrow 0$ we have $\mathcal{N}'_2 = 0$ from Eq. (7.106), so $\mathcal{N}_2 = \text{constant}$ for neutrinos. For photons, Θ_2 decreases due to the collision term on the right hand side of Eq. (7.81). Neglecting the contributions of photons on the right hand side of Eq. (7.109) and using the Friedmann equation $3\mathcal{H}^2 = 8\pi G a^2(\rho_\gamma + \rho_\nu)$, we obtain

$$\mathcal{N}_2 = -\frac{k^2(\Psi + \Phi)}{12r_\nu\mathcal{H}^2}, \quad r_\nu = \frac{\rho_\nu}{\rho_\gamma + \rho_\nu}. \quad (7.124)$$

Setting $l = 2$ in Eq. (7.106), we obtain $\mathcal{N}'_2 + (k/5)(3\mathcal{N}_3 - 2\mathcal{N}_1) = 0$. Taking the η derivative of this equation, using Eq. (7.105), and neglecting the contribution from $\mathcal{N}'_3$, we find

$$\mathcal{N}''_2 = \frac{2}{15}k^2(\mathcal{N}_0 + \Psi - 2\mathcal{N}_2). \quad (7.125)$$

For $\mathcal{N}_2 = 0$, we have shown that Φ and Ψ are constants. Now, we deal with $\mathcal{N}_2$ as a perturbation for the zeroth order solution $\Psi = -\Phi$. Setting $\Phi' = 0$ in Eq. (7.118),

it follows that $\Psi = -2\Theta_0 = -2\mathcal{N}_0$. In Eq. (7.124) we can deal with the term $\mathcal{C} = -k^2(\Psi + \Phi)/(12r_\nu)$ as constants, so differentiating the relation $\mathcal{N}_2 = \mathcal{C}\mathcal{H}^{-2}$ twice with respect to η in the radiation era ($a \propto \eta$) gives $\mathcal{N}_2 = 2\mathcal{C} = -k^2(\Psi + \Phi)/(6r_\nu)$. Using this relation with Eq. (7.125) and finally taking the limit $k \rightarrow 0$, we obtain

$$\Phi = -\left(1 + \frac{2}{5}r_\nu\right)\Psi. \quad (7.126)$$

This means that, in the presence of neutrino anisotropic stress, Eq. (7.120) is modified to

$$\Psi(0) = -2\Theta_0(0), \quad \Phi(0) = 2\Theta_0(0)\left(1 + \frac{2}{5}r_\nu\right). \quad (7.127)$$

From Eq. (2.17) the energy density of photons is given by $\rho_\gamma = \pi^2 T_\gamma^4/15$, whereas for neutrinos with three flavors we have $\rho_\nu = 7\pi^2 T_\nu^4/40$ from Eq. (4.60). From Eq (4.58) there is the relation $T_\nu = (4/11)^{1/3}T_\gamma$ after the annihilation of electrons and positrons, so that $r_\nu \simeq 0.405$. Compared to the case in which the anisotropic stress is ignored, $\Phi(0)$ is subject to change by 16%. After the radiation era the anisotropic stress of neutrinos can be neglected, and hence $\Psi \simeq -\Phi$.

7.6. Evolution of gravitational potentials

After the Universe enters the matter-dominated epoch, the gravitational clustering of non-relativistic matter starts to occur due to the decrease of the radiation pressure. We estimate the comoving wavenumber $k_{\text{eq}} = a_{\text{eq}}H(a_{\text{eq}})$ at which the radiation and matter densities are equivalent to each other (characterized by the scale factor a_{eq}). Since the Hubble parameter is given by $H(a_{\text{eq}}) = H_0\sqrt{2\Omega_m^{(0)}/a_{\text{eq}}^3}$ at $a = a_{\text{eq}}$, we obtain

$$k_{\text{eq}} = H_0\sqrt{\frac{2\Omega_m^{(0)}}{a_{\text{eq}}}} \simeq 0.073\Omega_m^{(0)}h^2\text{Mpc}^{-1}, \quad (7.128)$$

where $H_0^{-1} \simeq 3000h^{-1}\text{Mpc}$. For the perturbations whose physical wavelengths are larger than the order of 100 Mpc, they enter the Hubble radius for a larger than a_{eq} .

Let us consider the perturbations with the comoving wavenumber k much smaller than k_{eq} . For the perturbations outside the Hubble radius ($k < \mathcal{H}$), the relations (7.114) and (7.115) approximately hold during the matter era. For the system of non-relativistic matter and radiation, Eq. (7.107) reads

$$3\mathcal{H}(\Phi' - \mathcal{H}\Psi) \simeq 4\pi G a^2(\rho_m\delta_m + 4\rho_\gamma\Theta_0 + 4\rho_\nu\mathcal{N}_0). \quad (7.129)$$

We express Θ_0 and $\mathcal{N}_0$ in terms of δ_m by using the adiabatic solution (7.117) and introduce the dimensionless quantity $y = a/a_{\text{eq}} = \rho_m/\rho_r$. On using

$3\mathcal{H}^2 = 8\pi G a^2 \rho_r(y+1)$, Eq. (7.129) reduces to

$$y \frac{d\Phi}{dy} - \Psi = \frac{3y+4}{6(y+1)} \delta_m. \quad (7.130)$$

We neglect the contribution of the neutrino anisotropic stress and set $\Psi = -\Phi$. Differentiating Eq. (7.130) with respect to y , it follows that

$$\frac{d^2\Phi}{dy^2} + \frac{21y^2 + 54y + 32}{2y(y+1)(3y+4)} \frac{d\Phi}{dy} + \frac{1}{y(y+1)(3y+4)} \Phi = 0. \quad (7.131)$$

The solution to this equation can be written as

$$\Phi(y) = C_1 \frac{\sqrt{y+1}}{y^3} + C_2 \frac{9y^3 + 2y^2 - 8y - 16}{y^3}, \quad (7.132)$$

where C_1 and C_2 are integration constants. Under the initial conditions $\Phi = \Phi(0)$ and $\Phi'(0) = 0$, it follows that $C_1 = 16C_2 = 8\Phi(0)/5$. This leads to the following solution:

$$\Phi(y) = \Phi(0) \frac{9y^3 + 2y^2 - 8y - 16 + 16\sqrt{y+1}}{10y^3}. \quad (7.133)$$

In the limit that $y \rightarrow \infty$, we have $\Phi(y) \rightarrow 9\Phi(0)/10$. During the transition from the radiation era to the matter era, the gravitational potential Φ decreases by 10%.

We also consider the evolution of perturbations for the modes $k \gg k_{\text{eq}}$ during the radiation dominance. They enter the Hubble radius for the scale factor a much smaller than a_{eq} . Ignoring the term $\rho_m \delta_m$ and the anisotropic stress relative to $\rho_r \Theta_{r,0}$ in Eqs. (7.107) and (7.110) and combining them to eliminate the term $\rho_r \Theta_{r,0}$, it follows that

$$\Phi'' + 3\mathcal{H}\Phi' - \mathcal{H}\Psi' + \frac{1}{3}k^2\Phi - 2(\mathcal{H}^2 + \mathcal{H}')\Psi = 0, \quad (7.134)$$

where $\mathcal{H} = 1/\eta$ during the radiation era. Neglecting the neutrino anisotropic stress and using the solution $\Psi = -\Phi$, we obtain

$$\Phi'' + \frac{4}{\eta}\Phi' + \frac{1}{3}k^2\Phi = 0, \quad (7.135)$$

whose solutions are given by $[\sqrt{3} \sin(k\eta/\sqrt{3}) \pm k\eta \cos(k\eta/\sqrt{3})]/\eta^3$. The solution approaching the constant $\Phi(0)$ in the early radiation era ($\eta \rightarrow 0$) yields

$$\Phi(\eta) = \frac{9\Phi(0)}{(k\eta)^3} \left[\sqrt{3} \sin\left(\frac{k\eta}{\sqrt{3}}\right) - k\eta \cos\left(\frac{k\eta}{\sqrt{3}}\right) \right], \quad (7.136)$$

which means that Φ exhibits a damped oscillation.

In the above discussion, we have shown that the gravitational potential stays with a constant value $9\Phi(0)/10$ for the modes $k < \mathcal{H}$ in the matter era. In the following, we will study the evolution of Φ for the modes $k > \mathcal{H}$ in the matter era. For baryon perturbations, we employ the approximation that the right hand side

of Eq. (7.98) vanishes due to the decrease of the electron number density n_e . The CDM perturbations obey Eqs. (7.99) and (7.100), so the perturbation equations of baryons and CDM can be written in a unified way, as

$$\delta'_m - k^2 v_m + 3\Phi' = 0, \quad (7.137)$$

$$v'_m + \mathcal{H}v_m + \Psi = 0. \quad (7.138)$$

Now, we rewrite the η derivative in terms of the $\mathcal{N} = \ln a$ derivative, as $\delta'_m = \mathcal{H}(d\delta_m/d\mathcal{N})$. Differentiating Eq. (7.137) with respect to $\mathcal{N}$ and using Eq. (7.138), it follows that

$$\frac{d^2\delta_m}{d\mathcal{N}^2} + \left(2 + \frac{\dot{H}}{H^2}\right) \frac{d\delta_m}{d\mathcal{N}} + \left(\frac{k}{\mathcal{H}}\right)^2 \Psi = -3 \left[\frac{d^2\Phi}{d\mathcal{N}^2} + \left(2 + \frac{\dot{H}}{H^2}\right) \frac{d\Phi}{d\mathcal{N}} \right]. \quad (7.139)$$

For the modes deep inside the Hubble radius ($k \gg \mathcal{H}$), the left hand side of Eq. (7.107) is approximated as $k^2\Phi$. During the matter era, the contribution of radiation perturbations on the right hand side of Eq. (7.107) can be neglected, so we find

$$\left(\frac{k}{\mathcal{H}}\right)^2 \Phi \simeq \frac{3}{2} \Omega_m \delta_m, \quad (7.140)$$

where $\Omega_m = 8\pi G\rho_m/(3H^2)$. We use the approximation $\Psi \simeq -\Phi$ by ignoring the anisotropic stress of radiation. For sub-Hubble perturbations, we can neglect the right hand side of Eq. (7.139) relative to the left hand side of it, and hence

$$\frac{d^2\delta_m}{d\mathcal{N}^2} + \left(2 + \frac{\dot{H}}{H^2}\right) \frac{d\delta_m}{d\mathcal{N}} - \frac{3}{2} \Omega_m \delta_m \simeq 0. \quad (7.141)$$

From Eqs. (4.15) and (4.19), we have $\dot{H}/H^2 = -3/2$ during the matter dominance ($\Omega_m \simeq 1$). Substituting $\delta_m = e^{\lambda\mathcal{N}}$ into Eq. (7.141), we obtain two independent solutions $\lambda = 1, -3/2$ in the matter era. The growing-mode solution corresponds to $\lambda = 1$, i.e.,

$$\delta_m \propto a \propto t^{2/3}. \quad (7.142)$$

Substituting the solution (7.142) into Eq. (7.140), the evolution of gravitational potentials is given by

$$\Phi \simeq -\Psi \simeq \text{constant}. \quad (7.143)$$

The variations of Φ and Ψ start to occur after the Universe enters the epoch of cosmic acceleration.

For perturbations whose comoving wavenumber is of the order of k_{eq} , we need to solve the perturbation equations of motion numerically. In the flat Λ CDM model

there is the relation $\Omega_m = 1 - \Omega_r - \Omega_\Lambda$, where Ω_r , Ω_m , and Ω_Λ are the density parameters of radiation, non-relativistic matter, and the cosmological constant, respectively. Each matter component obeys the continuity equation (4.20) with the equation of state: $w = 1/3$ (radiation), $w = 0$ (non-relativistic matter), and $w = -1$ (cosmological constant). Using Eq. (4.19) as well, we obtain the differential equations

$$\frac{d\Omega_r}{d\mathcal{N}} = -(1 + 3\Omega_\Lambda - \Omega_r)\Omega_r, \quad (7.144)$$

$$\frac{d\Omega_\Lambda}{d\mathcal{N}} = (3 - 3\Omega_\Lambda + \Omega_r)\Omega_\Lambda, \quad (7.145)$$

$$\frac{d\mathcal{H}}{d\mathcal{N}} = -\frac{1}{2}(1 - 3\Omega_\Lambda + \Omega_r)\mathcal{H}. \quad (7.146)$$

Neglecting the term $\rho_r\Theta_{r,2}$ in Eqs. (7.109) and (7.110) and combining Eqs. (7.107) and (7.110) to eliminate the term $\rho_r\Theta_{r,0}$, it follows that

$$\frac{d^2\Phi}{d\mathcal{N}^2} + \left(4 + \frac{1}{\mathcal{H}} \frac{d\mathcal{H}}{d\mathcal{N}}\right) \frac{d\Phi}{d\mathcal{N}} + \left[2 + \frac{2}{\mathcal{H}} \frac{d\mathcal{H}}{d\mathcal{N}} + \frac{1}{3} \left(\frac{k}{\mathcal{H}}\right)^2\right] \Phi - \frac{1}{2}\Omega_m\delta_m \simeq 0. \quad (7.147)$$

Under the condition that the main contribution to δ_m comes from the CDM perturbation, we need to solve Eqs. (7.99) and (7.100) by coupling them with Eqs. (7.144)–(7.147). As estimated by Eqs. (7.120), (7.121) and (7.123), the adiabatic initial conditions correspond to $\delta_c(0) = 3\Phi(0)/2$ and $v_c = \Phi(0)/(2\mathcal{H})$.

In Fig. 7.1, we plot the evolution of Φ for three different values of k . From Eq. (2.10) the comoving wavenumber k_0 associated with the today's Hubble radius H_0^{-1} corresponds to $k_0 = H_0 = 2.3 \times 10^{-4} \text{ Mpc}^{-1}$ for $h = 0.7$. In the case (a) of Fig. 7.1, the comoving wavenumber is much smaller than k_{eq} , so the value of Φ in the matter era is 9/10 times as large as that in the radiation era. During the matter era, Φ stays nearly constant, but it starts to decay after the onset of cosmic acceleration. In the case (b), which corresponds to $k = k_{\text{eq}} = 160H_0$, the decrease of Φ during the transition to the matter era is more significant compared to the case (b). In the case (c), the comoving wavenumber is much larger than k_{eq} , so Φ exhibits a damped oscillation as estimated by Eq. (7.136).

Since the evolution of Φ is different depending on the values of k , we introduce a transfer function $T(k)$ to quantify the scale dependence. Given that the gravitational potential Φ of a super-Hubble mode ($k < \mathcal{H}$) approaches a constant at a scale factor a_m in the matter era, we denote the value of Φ at $a = a_m$ as $\Phi_{\text{LS}}(k, a_m)$. The transfer function is defined as $T(k) = \Phi(k, a_m)/\Phi_{\text{LS}}(k, a_m)$, where $\Phi(k, a_m)$ is the value of Φ for arbitrary wavenumbers k at $a = a_m$. The transfer function $T(k)$ is determined by numerically solving the perturbation equations of motion for each k . The appropriate choice of $T(k)$ is known as the following Bardeen-Bond-Kaiser-Szalay

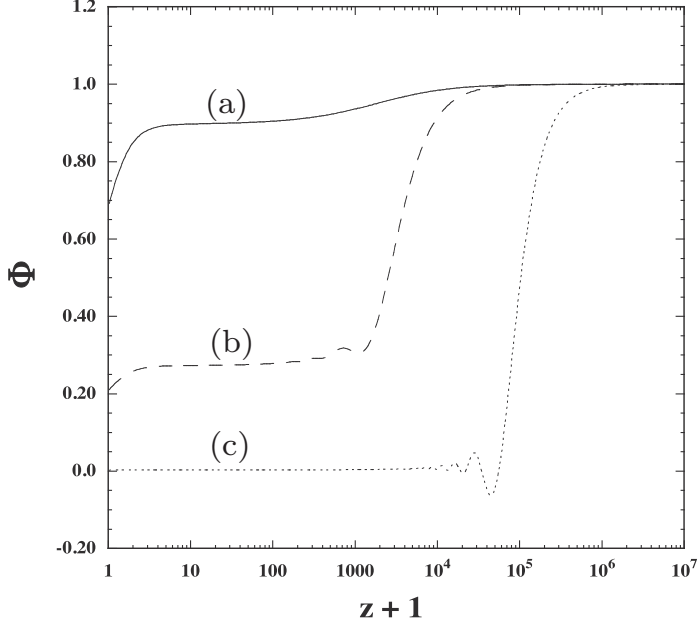


Fig. 7.1. Evolution of the gravitational potential Φ in the Λ CDM model from the radiation era to today. The present epoch ($z = 0$) is identified by $\Omega_m^{(0)} = 0.27$ and $\Omega_r^{(0)} = 9.4 \times 10^{-5}$, with $h = 0.7$. Each line corresponds to (a) $k = 5.0 \times 10^{-4} \text{ Mpc}^{-1} \ll k_{\text{eq}}$, (b) $k = 3.7 \times 10^{-2} \text{ Mpc}^{-1} = k_{\text{eq}}$, and (c) $k = 1.0 \text{ Mpc}^{-1} \gg k_{\text{eq}}$.

(BBKS) transfer function [8]:

$$T(x) = \frac{\ln(1 + 0.171x)}{0.171x} [1 + 0.284x + (1.18x)^2 + (0.399x)^3 + (0.490x)^4]^{-1/4}, \quad (7.148)$$

where $x \equiv k/k_{\text{eq}}$. For $k \ll k_{\text{eq}}$ we have $T(k) \simeq 1$ and hence $\Phi(k, a_m) \simeq \Phi_{\text{LS}}(k, a_m)$. Since the transfer function $T(k)$ has the dependence $T(k) \propto \ln k/k^2$ for $k \gg k_{\text{eq}}$, $\Phi(k, a_m)$ tends to decrease for larger k .

As we see in Fig. 7.1, Φ starts to decrease after the onset of comic acceleration. In order to describe the evolution of Φ , we introduce the growth function $D(a)$ for $a > a_m$ and express the gravitational potential in the form $\Phi(a)/\Phi(a_m) = D(a)/a$. From Eq. (7.142), the growth function evolves as $D(a) \propto a$ during the matter dominance, but after dark energy dominates over non-relativistic matter, $D(a)$ is not proportional to a . From the above discussion, the gravitational potential for $a > a_m$ is given by

$$\Phi(k, a) = \Phi_{\text{LS}}(k, a_m) T(k) \frac{D(a)}{a}. \quad (7.149)$$

We recall that there is the relation (6.124) between the gravitational potentials Φ , Ψ and the curvature perturbation $\mathcal{R}$. If $\Phi' \simeq 0$ and $\Psi \simeq -\Phi$ during the matter

era, this relation reduces to Eq. (6.125). Then, curvature perturbation $\mathcal{R}(k, a_i)$ generated during inflation is related to the gravitational potential $\Phi_{\text{LS}}(k, a_m)$ in the matter era, as $\mathcal{R}(k, a_i) = (5/3)\Phi_{\text{LS}}(k, a_m)$. Then, today's gravitational potential (at $a_0 = 1$) is expressed as

$$\Phi(k, a_0) = \frac{3}{5}\mathcal{R}(k, a_i)T(k)D(a_0). \quad (7.150)$$

The primordial power spectrum $P_{\mathcal{R}}(k) = \langle \mathcal{R}^2(k, a_i) \rangle$ generated during inflation is given by Eq. (6.174). We employ the primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k) = k^3 P_{\mathcal{R}}(k)/(2\pi^2)$ and introduce its amplitude $\mathcal{P}_{\mathcal{R}}(k_0)$ and the scalar spectral index n_s as Eq. (6.181), where k_0 is a pivot wavenumber. Since $P_{\mathcal{R}}(k, a_i) = (2\pi^2/k^3)\mathcal{P}_{\mathcal{R}}(k_0)(k/k_0)^{n_s-1}$, today's power spectrum $P_{\Phi} = \langle \Phi^2(k, a_0) \rangle$ of the gravitational potential yields

$$P_{\Phi}(a_0) = \frac{18\pi^2}{25} \frac{\mathcal{P}_{\mathcal{R}}(k_0)}{k_0^{n_s-1}} k^{n_s-4} T^2(k) D^2(a_0). \quad (7.151)$$

This will be used for the computation of large-scale CMB temperature anisotropies in Sec. 7.10.

7.7. Angular power spectrum of CMB temperature anisotropies

The CMB temperature anisotropy Θ is a two-dimensional observable defined on the celestial sphere, so we expand it on the basis of spherical harmonics Y_l^m . This expansion is given by Eq. (7.67), whose coefficient a_{lm} characterizes the amplitude of perturbations. On using Eq. (7.67) with the normalization (7.68) of Y_l^m , it follows that

$$a_{lm} = \int d\Omega \Theta(\mathbf{n}) Y_l^{m*}(\mathbf{n}). \quad (7.152)$$

Taking the product of a_{lm} and $a_{l'm'}^*$, we have

$$\langle a_{lm} a_{l'm'}^* \rangle = \int d\Omega \int d\Omega' Y_l^{m*}(\mathbf{n}) Y_{l'}^{m'}(\mathbf{n}') w(\theta), \quad (7.153)$$

where $w(\theta) = \langle \Theta(\mathbf{n}) \Theta(\mathbf{n}') \rangle$ is a function that depends on the angle θ between $\mathbf{n}$ and $\mathbf{n}'$. We expand this function in terms of the Legendre polynomials $\mathcal{P}_l(\cos\theta)$, as

$$w(\theta) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} C_l \mathcal{P}_l(\cos\theta). \quad (7.154)$$

Substituting Eq. (7.70) into Eq. (7.154) and using the fact that the range of m is $-l \leq m \leq l$, we have

$$w(\theta) = \sum_{l=0}^{\infty} \sum_{m=-l}^l C_l Y_l^m(\mathbf{n}) Y_l^{m*}(\mathbf{n}'). \quad (7.155)$$

Plugging Eq. (7.155) into Eq. (7.153) and using Eq. (7.68), we obtain the orthogonal relation

$$\langle a_{lm} a_{l'm'}^* \rangle = C_l \delta_{ll'} \delta_{mm'}, \quad (7.156)$$

where C_l is called the angular power spectrum characterizing the amplitude of temperature fluctuations. From Eq. (7.156), we can express C_l as

$$C_l = \frac{1}{2l+1} \sum_{m=-l}^l \langle |a_{lm}|^2 \rangle. \quad (7.157)$$

Expanding Θ_l into the Fourier series, as $\Theta_l = \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} \Theta_l(\mathbf{k})$, and taking note that a_{lm} is related to Θ_l according to Eq. (7.72), we obtain

$$a_{lm} = 4\pi (-i)^l \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} \Theta_l(\mathbf{k}) Y_l^{m*}(\hat{\mathbf{k}}). \quad (7.158)$$

Employing Eq. (7.70) and computing C_l in Eq. (7.157), we find

$$C_l = 4\pi \int \frac{d^3 k}{(2\pi)^3} \int \frac{d^3 k'}{(2\pi)^3} \langle \Theta_l^*(\mathbf{k}) \Theta_l(\mathbf{k}') \rangle e^{-i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{x}} \mathcal{P}_l(\cos \tilde{\theta}), \quad (7.159)$$

where $\tilde{\theta}$ is the angle between $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$. We define the power spectrum P_{Θ_l} associated with Θ_l , as

$$\langle \Theta_l^*(\mathbf{k}) \Theta_l(\mathbf{k}') \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{k} - \mathbf{k}') P_{\Theta_l}. \quad (7.160)$$

On using $\mathcal{P}_l(1) = 1$, we can express C_l in the form

$$C_l = \frac{2}{\pi} \int_0^\infty dk k^2 P_{\Theta_l}(k). \quad (7.161)$$

Provided that the present value of $\Theta_l(\mathbf{k}, a_0)$ is known for each Fourier mode $\mathbf{k}$, we can derive $C_l(a_0)$ according to the integral (7.161).

The integer l appearing in the expansion of temperature fluctuations in terms of Y_l^m can be interpreted as the comoving wavenumber $\mathbf{k}$ with respect to the basis $e^{i\mathbf{k} \cdot \mathbf{x}}$. The smaller multipole l corresponds to the larger angle θ . For the angle θ measured by observers, there is the approximate relation $l \approx \pi/\theta$. The WMAP and Planck satellites measured C_l in the ranges $2 \leq l \lesssim 1000$ and $2 \leq l \lesssim 2500$, respectively. In the flat FLRW Universe, the comoving distance from today ($\eta = \eta_0$) to the CMB decoupling epoch ($\eta = \eta_*$) is given by $r = \eta_0 - \eta_* \approx \eta_0$. The distance $\lambda \approx \pi/k$ between the two points on the CMB celestial sphere is measured as the angle $\theta = \lambda/r$, so there is the following relation between k and l :

$$k \approx \frac{l}{\eta_0}. \quad (7.162)$$

Since $\eta_0 \approx H_0^{-1}$, the largest scales observed in CMB measurements are the wavelengths of the order of H_0^{-1} .

7.8. Evolution of photon perturbations in the tight coupling era

In this section, we study the evolution of perturbations in the epoch where photons and baryons are tightly coupled with each other before the CMB decoupling epoch. In this regime, the optical depth defined by Eq. (7.83) is much larger than 1. From Eq. (7.84) we can ignore higher-order terms of Θ_l with $l \geq 2$ in the tight-coupling limit, so we only consider the monopole Θ_0 and the dipole Θ_1 .

The sound speed squared for the coupled system of photons and baryons is given by $c_s^2 = \delta P_\gamma / (\delta \rho_\gamma + \delta \rho_b)$. We assume that photons and baryons are perfect fluids satisfying the adiabatic condition $\delta \rho_\gamma / \rho_\gamma = (4/3) \delta \rho_b / \rho_b$. Then, the sound speed squared yields

$$c_s^2 = \frac{1}{3(1 + R_s)}, \quad R_s = \frac{3\rho_b}{4\rho_\gamma}. \quad (7.163)$$

Without baryons we have $c_s^2 = 1/3$, but the existence of baryons leads to smaller c_s^2 . On using τ and R_s , we can write Eq. (7.98) in the form

$$v_b - v_\gamma = \frac{R_s}{\tau'} (v'_b + \mathcal{H}v_b + \Psi). \quad (7.164)$$

In the tight-coupling regime ($|\tau'| \gg 1$) the right hand side of Eq. (7.164) is close to 0, so that $v_b \simeq v_\gamma = -3\Theta_1/k$ at zeroth order. Substituting this relation into the right hand side of Eq. (7.164), we obtain

$$v_b \simeq -\frac{3}{k} \left[\Theta_1 + \frac{R_s}{\tau'} \left(\Theta'_1 + \mathcal{H}\Theta_1 - \frac{k}{3}\Psi \right) \right]. \quad (7.165)$$

Ignoring the contribution Θ_2 relative to Θ_0 in Eq. (7.80), it follows that

$$\Theta'_1 - \frac{k}{3}(\Theta_0 + \Psi) \simeq \tau' \left(\Theta_1 + \frac{1}{3}k v_b \right). \quad (7.166)$$

From Eq. (7.79) we have

$$\Theta_1 = -\frac{1}{k}(\Theta'_0 + \Phi'). \quad (7.167)$$

Plugging Eqs. (7.165) and (7.167) into Eq. (7.166), we find

$$\Theta'_1 \simeq \frac{1}{k} \left[c_s^2 k^2 \Theta_0 + 3\mathcal{H}c_s^2 R_s (\Theta'_0 + \Phi') + \frac{k^2}{3}\Psi \right]. \quad (7.168)$$

Taking the η derivative of Eq. (7.79) leads to $\Theta''_0 + k\Theta'_1 + \Phi'' = 0$. Substituting Eq. (7.168) into this relation, we obtain

$$\left(\frac{d^2}{d\eta^2} + 3\mathcal{H}c_s^2 R_s \frac{d}{d\eta} + k^2 c_s^2 \right) (\Theta_0 + \Phi) = k^2 \left(c_s^2 \Phi - \frac{1}{3}\Psi \right). \quad (7.169)$$

The second term on the left hand side of Eq. (7.169) is of the order of $\mathcal{H}^2 c_s^2 R_s (\Theta_0 + \Phi)$, so it can be neglected relative to the third term under the condition $R_s \ll$

$k^2/\mathcal{H}^2$. Provided that $R_s \ll 1$, the condition $R_s \ll k^2/\mathcal{H}^2$ holds for perturbations inside the Hubble radius. Approximating $c_s^2 \simeq 1/3$ on the right hand side of Eq. (7.169), it follows that

$$\left(\frac{d^2}{d\eta^2} + k^2 c_s^2 \right) (\Theta_0 + \Phi) \simeq \frac{k^2}{3} (\Phi - \Psi). \quad (7.170)$$

The general solution to Eq. (7.170) is expressed in terms of the sum of a homogenous solution (derived by setting the right hand side of Eq. (7.170) to zero) and a special solution. Defining the sound horizon, as

$$r_s(\eta) = \int_0^\eta d\tilde{\eta} c_s(\tilde{\eta}), \quad (7.171)$$

the homogenous solution is the linear combination of two functions:

$$f_1(\eta) = \sin[kr_s(\eta)], \quad f_2(\eta) = \cos[kr_s(\eta)]. \quad (7.172)$$

The special solution to Eq. (7.170) can be derived by using the method of Green functions. In this way, we obtain the general solution to Eq. (7.170), as

$$\begin{aligned} \Theta_0(\eta) + \Phi(\eta) &= c_1 f_1(\eta) + c_2 f_2(\eta) \\ &+ \frac{k^2}{3} \int_0^\eta d\tilde{\eta} [\Phi(\tilde{\eta}) - \Psi(\tilde{\eta})] \frac{f_1(\tilde{\eta})f_2(\eta) - f_1(\eta)f_2(\tilde{\eta})}{f_1(\tilde{\eta})f_2'(\tilde{\eta}) - f_1'(\tilde{\eta})f_2(\tilde{\eta})}, \end{aligned} \quad (7.173)$$

where c_1 and c_2 are constants. Under the adiabatic initial condition we have $\Theta_0 + \Phi = \text{constant}$ at $\eta = 0$, so the coefficient c_1 is fixed as $c_1 = 0$. Then, Eq. (7.173) reduces to

$$\begin{aligned} \Theta_0(\eta) + \Phi(\eta) &= [\Theta_0(0) + \Phi(0)] \cos(kr_s) \\ &+ \frac{k}{\sqrt{3}} \int_0^\eta d\tilde{\eta} [\Phi(\tilde{\eta}) - \Psi(\tilde{\eta})] \sin[k(r_s(\eta) - r_s(\tilde{\eta}))]. \end{aligned} \quad (7.174)$$

This result is valid before the CMB decoupling epoch ($\eta = \eta_*$), which can be used for the estimation of the monopole component Θ_0 at $\eta = \eta_*$. In the case where the first term on the right hand side of Eq. (7.174) dominates over the second term, $\Theta_0(\eta_*) + \Phi(\eta_*)$ has peaks at

$$kr_s(\eta_*) = n\pi, \quad (7.175)$$

where $n = 1, 2, 3, \dots$. The peaks arise due to acoustic oscillations of the photon-baryon fluid induced by the term $k^2 c_s^2$ on the left hand side of Eq. (7.170).

The scale $\lambda = \pi/k$ associated with the first peak ($n = 1$) corresponds to the sound horizon $r_s(\eta_*)$. The comoving angular diameter distance $D_A(\eta_*)$ to the last scattering surface is related to the length scale $r_s(\eta_*)$ and the associated angle θ_A

measured by the observer, as $r_s(\eta_*) = D_A(\eta_*)\theta_A$. The multipole l corresponding to θ_A is given by

$$l_A \equiv \frac{\pi}{\theta_A} = \pi \frac{D_A(\eta_*)}{r_s(\eta_*)}. \quad (7.176)$$

From Eqs. (7.171) and (7.163), we can express $r_s(\eta_*)$ as

$$r_s(\eta_*) = \frac{1}{\sqrt{3}H_0} \int_0^{a_*} \frac{da}{\sqrt{1 + R_s(a)} a^2 E(a)}, \quad (7.177)$$

where $E(a) = H(a)/H_0$, and we have changed the variable η to a by using the relation $d\eta = da/(a^2 H)$. The evolution of E for $z > z_*$ is given by $E(a) = (\sqrt{a + a_{\text{eq}}}/a^2) \sqrt{\Omega_m^{(0)}}$, where $a_{\text{eq}} = (1 + z_{\text{eq}})^{-1}$ is the value of a at the radiation-matter equality. Defining the quantities $\omega_i = \Omega_i^{(0)} h^2$, where $i = \gamma, b, m$, we can express $R_s(a)$ in the form $R_s(a) = (3\omega_b/4\omega_\gamma)a$. Then, Eq. (7.177) is integrated to give

$$r_s(\eta_*) = \frac{4}{3} \frac{h}{H_0} \sqrt{\frac{\omega_\gamma}{\omega_m \omega_b}} \ln \left(\frac{\sqrt{R_s(a_*) + R_s(a_{\text{eq}})} + \sqrt{1 + R_s(a_*)}}{1 + \sqrt{R_s(a_{\text{eq}})}} \right). \quad (7.178)$$

The comoving angular diameter distance D_A , which corresponds to the division of the angular diameter distance d_A in Eq. (4.9) with respect to $a(t)$, is equivalent to $f_K(\chi)$ in Eq. (4.5). As for the light propagation in the χ direction, the comoving distance from the CMB decoupling epoch to today is given by $\chi = \int_0^{z_*} dz/H(z)$, see Eq. (4.8). Substituting this into Eq. (4.5) and using the density parameter $\Omega_K^{(0)} = -K/H_0^2$ of spatial curvature, we obtain

$$D_A(\eta_*) = \frac{\mathcal{R}_{\text{CMB}}}{H_0 \sqrt{\Omega_m^{(0)}}}, \quad (7.179)$$

where

$$\mathcal{R}_{\text{CMB}} = \sqrt{\frac{\Omega_m^{(0)}}{\Omega_K^{(0)}}} \sinh \left(\sqrt{\Omega_K^{(0)}} \int_0^{z_*} \frac{dz}{E(z)} \right). \quad (7.180)$$

From Eqs. (7.178) and (7.179), the multipole l_A in Eq. (7.176) yields

$$l_A = \frac{3\pi}{4} \sqrt{\frac{\omega_b}{\omega_\gamma}} \mathcal{R}_{\text{CMB}} \left[\ln \left(\frac{\sqrt{R_s(a_*) + R_s(a_{\text{eq}})} + \sqrt{1 + R_s(a_*)}}{1 + \sqrt{R_s(a_{\text{eq}})}} \right) \right]^{-1}. \quad (7.181)$$

The quantity $\mathcal{R}_{\text{CMB}}$ is called the CMB shift parameter [9]. Under the change of $H(z)$ from $z = z_*$ to today ($z = 0$), the position of l_A is subject to change. From the

Planck 2015 data, the CMB shift parameter and the multipole l_A were constrained to be $\mathcal{R}_{\text{CMB}} = 1.7488 \pm 0.0074$ and $l_A = 301.76 \pm 0.14$ by assuming the standard cosmology with a constant dark energy equation of state [10].

As we will see in Sec. 7.10, the positions of CMB acoustic peaks are shifted toward larger scales from the contributions higher than the monopole Θ_0 and the free streaming of photons from the decoupling epoch to today. The position of the first acoustic peak is around $l \simeq 200$. As we will discuss in Sec. 7.9, a phenomenon called the Silk damping leads to the suppression of $\Theta_0(\eta_*) + \Phi(\eta_*)$ than that estimated by Eq. (7.174).

Substituting Eq. (7.174) into Eq. (7.167), we obtain

$$\begin{aligned} \Theta_1(\eta) = & \frac{1}{\sqrt{3}} [\Theta_0(0) + \Phi(0)] \sin(kr_s) \\ & - \frac{k}{3} \int_0^\eta d\tilde{\eta} [\Phi(\tilde{\eta}) - \Psi(\tilde{\eta})] \cos[k(r_s(\eta) - r_s(\tilde{\eta}))]. \end{aligned} \quad (7.182)$$

The phase of the first term on the right hand side of Eq. (7.182) is different from that of the first term on the right hand side of Eq. (7.174) by the factor $\pi/2$, so the dipole component gives rise to the phase contribution different from that of the multipole component.

7.9. Silk damping

The mean free path of photons $\ell_\gamma = 1/(n_e \sigma_T)$ is related to τ defined by Eq. (7.83). For larger ℓ_γ , τ tends to be smaller. For the perturbation whose wavelength is much smaller than the Hubble radius ($k \gg aH$), we cannot ignore the terms higher than $l = 1$. In this section, we show that inclusion of the term $\Theta_2 = k^2 \Pi_\gamma / (4\rho_\gamma)$ leads to a suppression of the amplitude of temperature fluctuations on small scales, which is called diffusion damping or Silk damping [11].

In the strong-coupling regime, we define a small parameter $\epsilon_c \equiv -1/\tau' = (n_e \sigma_T a)^{-1}$ corresponding to the inverse of τ' . Moreover, for the perturbation whose wavelength is much smaller than the Hubble radius, we can set $\Phi' = 0$ in Eqs. (7.91) and (7.97), so that

$$v_\gamma \simeq \frac{3\delta'_\gamma}{4k^2}, \quad v_b \simeq \frac{\delta'_b}{k^2}. \quad (7.183)$$

From Eqs. (7.92) and (7.98), we obtain

$$v_b - v_\gamma \simeq \epsilon_c (v'_\gamma + \delta_\gamma/4 - 2\Theta_2), \quad (7.184)$$

$$v'_\gamma + \frac{1}{4}\delta_\gamma - 2\Theta_2 \simeq -R_s v'_b, \quad (7.185)$$

where we have set $\Psi = 0$ and ignored the term $\mathcal{H}v_b$ relative to v'_b . From Eq. (7.81), it follows that

$$\Theta_2 = -\frac{10}{9}\epsilon_c \left[\Theta'_2 + \frac{k}{5} \left(3\Theta_3 + \frac{2}{3}kv_\gamma \right) \right], \quad (7.186)$$

where we used $\Theta_1 = -kv_\gamma/3$. We employ the approximation of expansion in terms of the small parameter ϵ_c one after another. At zeroth order of ϵ_c , we have that $v_b = v_\gamma$ and $\Theta_2 = 0$. At first order in ϵ_c , there is the difference between v_b and v_γ . Substitution of the zeroth order solution into Eq. (7.185) gives $v'_\gamma = -\delta_\gamma/[4(1+R_s)]$. Hence, from Eq. (7.184), we obtain

$$v_b = \frac{3\delta'_\gamma}{4k^2} + \frac{R_s\delta_\gamma}{4(1+R_s)}\epsilon_c. \quad (7.187)$$

At first order in ϵ_c , Eq. (7.186) gives

$$\Theta_2 = -\frac{4}{27}k^2v_\gamma\epsilon_c = -\frac{1}{9}\delta'_\gamma\epsilon_c. \quad (7.188)$$

At second order in ϵ_c , we substitute Eqs. (7.187) and (7.188) into Eq. (7.185) and employ Eq. (7.183). Then, we obtain the differential equation of δ_γ , as

$$\delta''_\gamma + f(\eta)\delta'_\gamma + c_s^2k^2\delta_\gamma = 0, \quad (7.189)$$

where

$$f(\eta) = \frac{k^2\epsilon_c}{3(1+R_s)} \left(\frac{8}{9} + \frac{R_s^2}{1+R_s} \right). \quad (7.190)$$

Since the time scales of the variations of R_s and ϵ_c are much larger than the time scale of oscillations of photons, we have ignored the terms $\dot{R}_s$ and $\dot{\epsilon}_c$. The damping of perturbations is induced by the second term of Eq. (7.189). To see this, we define the quantities $\beta(\eta) = \exp[\int f(\tilde{\eta}) d\tilde{\eta}]$ and $\tilde{\delta}_\gamma = \beta^{1/2}\delta_\gamma$. Then, Eq. (7.189) reduces to

$$\tilde{\delta}''_\gamma + \omega^2(\eta)\tilde{\delta}_\gamma = 0, \quad \omega^2(\eta) = c_s^2k^2 + \frac{\beta'^2}{4\beta^2} - \frac{\beta''}{2\beta}. \quad (7.191)$$

The solution to this equation is given by $\tilde{\delta}_\gamma \propto \exp[\pm i \int_0^\eta \omega(\tilde{\eta}) d\tilde{\eta}]$, so that

$$\delta_\gamma \propto \exp\left(-\frac{k^2}{k_D^2}\right) \exp\left[\pm i \int_0^\eta \omega(\tilde{\eta}) d\tilde{\eta}\right], \quad (7.192)$$

where

$$k_D^{-2} = \int_0^\eta d\tilde{\eta} \frac{1}{6(1+R_s)n_e\sigma_T a(\tilde{\eta})} \left(\frac{8}{9} + \frac{R_s^2}{1+R_s} \right). \quad (7.193)$$

For k larger than k_D , there is the exponential damping of photon perturbations. The solution (7.192) corresponds to the monopole mode $\Theta_0 = \delta_\gamma/4$. Since $\Theta_1 \simeq -\delta'_\gamma/(4k)$, the dipole moment Θ_1 also damps for $k > k_D$.

To estimate the damping scale, we first compute the electron density n_e . When photons were completely ionized long before the photon decoupling epoch, the proton number density n_p was equivalent to n_e by ignoring the contribution of helium. In reality, the helium with the mass fraction $Y_{\text{He}} \simeq 0.25$ exists [1, 2], so its ratio per nucleon relative to the total number density reads $Y_{\text{He}}/4$. Two protons inside a helium absorb two electrons, so the ratio of free electrons excluding absorbed electrons relative to the total number density (n_b) is given by $n_e = n_b(1 - Y_{\text{He}}/2)$. For the present baryon number density $n_b^{(0)}$, we have $n_b = n_b^{(0)}(a/a_0)^{-3}$ and $m_p n_b^{(0)}/\rho_0 = \Omega_b^{(0)}$, where $m_p = 1.67 \times 10^{-27}$ kg is the proton mass and $\rho_0 = 3H_0^2/(8\pi G)$ is the critical density. Then, the product of n_e and $\sigma_T = 6.65 \times 10^{-29} \text{ m}^2$ can be estimated as

$$n_e \sigma_T = 2.3 \times 10^{-5} \Omega_b^{(0)} h^2 (1 - Y_{\text{He}}/2) (a/a_0)^{-3} \text{ Mpc}^{-1}. \quad (7.194)$$

Approximating $R_s \simeq 0$ in Eq. (7.193), the right hand side of Eq. (7.193) can be integrated out. On using the relations $H = H_0[\Omega_m^{(0)}(1 + a_{\text{eq}}/a)]^{1/2}(a/a_0)^{-3/2}$ and $d\eta = da/(a^2 H)$, it follows that

$$k_D^{-1} = 4.4 \times 10^3 (\Omega_b^{(0)} h^2)^{-1/2} (\Omega_m^{(0)} h^2)^{-1/4} (1 - Y_{\text{He}}/2)^{-1/2} (a/a_0)^{5/4} \mathcal{F}(a/a_{\text{eq}}) \text{ Mpc}, \quad (7.195)$$

where

$$\mathcal{F}(x) = \left\{ \frac{2[\sqrt{x+1}(3x^2 - 4x + 8) - 8]}{15x^{5/2}} \right\}^{1/2}. \quad (7.196)$$

In the limit that $x \ll 1$, this function has the dependence $\mathcal{F}(x) \simeq x^{1/4}/\sqrt{3}$. For $a \ll a_{\text{eq}}$, k_D^{-1} increases in proportion to $a^{3/2}$. On using the values $Y_{\text{He}} = 0.25$, $\Omega_b^{(0)} = 0.022$, and $\Omega_m^{(0)} = 0.134$ for $a/a_0 = 10^{-4}$, we have $a/a_{\text{eq}} = 0.32$ from Eq. (4.80) and hence $k_D^{-1} \simeq 0.2 \text{ Mpc}$. The result (7.195) has been derived under the approximations (i) $R_s = 0$, and (ii) the ionization rate of electrons is 1, so the formula starts to lose its validity for the scale factor of the order of $a = 10^{-3} a_0$. Around the photon decoupling epoch, k_D^{-1} rapidly increases relative to the estimation (7.195) and the perturbations whose wavelengths are smaller than 10 Mpc are affected by the Silk damping.

7.10. Estimation of the CMB angular power spectrum and comparison with observations

We have discussed the evolution of perturbations up to the CMB decoupling epoch, but we need to study the evolution of Θ after the decoupling to compare the CMB temperature anisotropies with observations. In the following, we provide analytic estimations for today's temperature anisotropies. First, we can express Eq. (7.75)

in the form

$$e^{-i\mu k\eta+\tau} \frac{d}{d\eta} (\Theta e^{i\mu k\eta-\tau}) = F(\eta, \mu), \quad (7.197)$$

where

$$F(\eta, \mu) = -\Phi' - i\mu k\Psi - \tau' \left[\Theta_0 + i\mu k v_b - \frac{1}{2} \mathcal{P}_2(\mu) \Theta_2 \right]. \quad (7.198)$$

Integrating Eq. (7.197) from the initial time η_i to today (η_0) with respect to η , it follows that

$$\Theta(\eta_0) = e^{-i\mu k\eta_0+\tau(\eta_0)} \int_{\eta_i}^{\eta_0} d\eta F(\eta, \mu) e^{i\mu k\eta-\tau(\eta)} + \Theta(\eta_i) e^{i\mu k(\eta_i-\eta_0)} e^{-\tau(\eta_i)+\tau(\eta_0)}. \quad (7.199)$$

We can approximate today's optical depth as 0. On the other hand the optical depth $\tau(\eta_i)$ in the early Universe is much larger than 1, so it is a good approximation to ignore the second term on the right hand side of Eq. (7.199). Setting $\eta_i = 0$ in the integral of Eq. (7.199), we obtain

$$\Theta(\eta_0) = \int_0^{\eta_0} d\eta F(\eta, \mu) e^{i\mu k(\eta-\eta_0)-\tau(\eta)}. \quad (7.200)$$

On using Eq. (7.77), today's value of $\Theta_l(\eta)$ yields

$$\Theta_l(\eta_0) = i^l \int_0^{\eta_0} d\eta e^{-\tau(\eta)} \int_{-1}^1 \frac{d\mu}{2} e^{i\mu k(\eta-\eta_0)} F(\eta, \mu) \mathcal{P}_l(\mu). \quad (7.201)$$

Ignoring the last term $\mathcal{P}_2(\mu) \Theta_2/2$ of Eq. (7.198), the function $F(\eta, \mu)$ can be written in the form

$$F(\eta, \mu) = F_0(\eta) + F_1(\eta)\mu, \quad (7.202)$$

where $F_0(\eta) = -\Phi' - \tau'\Theta_0$ and $F_1(\eta) = -ik(\Psi + \tau'v_b)$.

The spherical Bessel function defined by

$$j_l(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\sin x}{x} \quad (7.203)$$

is related to the Legendre polynomials $\mathcal{P}_l(\mu)$, as

$$j_l(x) = i^l \int_{-1}^1 \frac{d\mu}{2} \mathcal{P}_l(\mu) e^{-i\mu x}. \quad (7.204)$$

Then, the contribution from $F_0(\eta)$ to Θ_l is given by

$$\Theta_{l,0}(\eta_0) = \int_0^{\eta_0} d\eta e^{-\tau(\eta)} F_0(\eta) j_l[k(\eta_0 - \eta)]. \quad (7.205)$$

As for the contribution $\Theta_{l,1}$ from $F_1(\eta)\mu$ to Θ_l , we perform the partial integration by using $e^{i\mu k(\eta-\eta_0)}\mu = (e^{i\mu k(\eta-\eta_0)})'/(ik)$. The boundary term $e^{-\tau(\eta_0)}F_1(\eta_0)$

appears after the integration, but this is the monopole moment that merely modifies the average temperature. Dropping such a contribution for the estimation of CMB fluctuations, it follows that

$$\Theta_{l,1}(\eta_0) = -\frac{1}{ik} \int_0^{\eta_0} d\eta (e^{-\tau(\eta)} F_1(\eta))' j_l[k(\eta_0 - \eta)]. \quad (7.206)$$

Then, we obtain

$$\Theta_l(\eta_0) = \int_0^{\eta_0} d\eta \mathcal{F}(\eta) j_l[k(\eta_0 - \eta)], \quad (7.207)$$

where

$$\mathcal{F}(\eta) = (\Theta_0 + \Psi)g(\eta) - [v_b g(\eta)]' + e^{-\tau}(\Psi' - \Phi'), \quad (7.208)$$

and

$$g(\eta) = -\tau' e^{-\tau}. \quad (7.209)$$

In the regimes $z \gg z_*$ and $z \ll z_*$, the function $g(\eta)$ is close to 0 due to the smallness of $e^{-\tau}$ and $-\tau'$, respectively. This function has a peak around $z = z_*$ with $g(\eta_*) \sim 0.02$. On using the fact that $g(\eta)$ has the property $\int_0^{\eta_0} d\eta g(\eta) = 1$ and dealing with $g(\eta)$ as a delta function having a peak around $\eta = \eta_*$, the contribution to $\Theta_l(\eta_0)$ coming from the first term on the right hand side of Eq. (7.208) can be estimated as $[\Theta_0(\eta_*) + \Psi(\eta_*)]j_l[k(\eta_0 - \eta_*)]$. As for the contribution to $\Theta_l(\eta_0)$ from the second term on the right hand side of Eq. (7.208), we perform the partial integration and use the property $(2l+1)dj_l(x)/dx = lj_{l-1}(x) - (l+1)j_{l+1}(x)$. We employ the approximate relation $v_b(\eta_*) = v_\gamma(\eta_*) = -3\Theta_1(\eta_*)/k$ and pick up the contributions around $\eta = \eta_*$. In summary, today's value of $\Theta_l(k, \eta_0)$ yields [4]

$$\begin{aligned} \Theta_l(k, \eta_0) &= [\Theta_0(k, \eta_*) + \Psi(k, \eta_*)]j_l[k(\eta_0 - \eta_*)] \\ &+ 3\Theta_1(k, \eta_*) \frac{lj_{l-1}[k(\eta_0 - \eta_*)] - (l+1)j_{l+1}[k(\eta_0 - \eta_*)]}{2l+1} \\ &+ \int_0^{\eta_0} d\eta e^{-\tau} [\Psi'(k, \eta) - \Phi'(k, \eta)]j_l[k(\eta_0 - \eta)], \end{aligned} \quad (7.210)$$

where we have explicitly written the k dependence of Θ_l .

The main contribution to $\Theta_l(k, \eta_0)$ corresponds to the values of Θ_0 , Θ_1 , and Ψ around $\eta = \eta_*$. The wavenumber k is related to l through the relation (7.162). If the gravitational potentials Ψ and Φ vary, the last integral of Eq. (7.210) contributes to the CMB temperature anisotropies. This is called the Integrated Sachs-Wolfe (ISW) effect. The ISW effect occurs when the gravitational potentials vary during the transition from the radiation era to the matter era and the transition from the matter era to the dark-energy dominated epoch.

Let us consider large-scale perturbations with the multipoles $l \lesssim 20$. Since the physical wavelength of perturbations is larger than the Hubble radius during most

of the cosmic expansion history, the amplitude of perturbations is frozen with the primordial value generated during inflation. For such large-scale perturbations, the dominant contribution to $\Theta_l(k, \eta_0)$ comes from the first term on the right hand side of Eq. (7.210). Then, we need to estimate the value of $\Theta_0 + \Psi$ at $\eta = \eta_*$. The relation (7.122) is valid for the modes $k \ll \mathcal{H}$ at $\eta = \eta_*$. As we discussed in Sec. 7.6, the initial value $\Phi(0)$ in the radiation era is related to the value $\Phi(\eta_*)$ at the CMB decoupling epoch, as $\Phi(0) = (10/9)\Phi(\eta_*)$. Then, we obtain the relation $\Theta_0(\eta_*) = 2\Phi(\eta_*)/3$. On using $\Psi \simeq -\Phi$ after the end of the radiation era, it follows that

$$\Theta_0(\eta_*) + \Psi(\eta_*) \simeq -\frac{1}{3}\Phi(\eta_*). \quad (7.211)$$

This relates the large-scale temperature anisotropy with the gravitational potential, which is dubbed the Sachs-Wolfe (SW) effect [12]. Since the photon reaches the observer in the gravitational field mediated by the potential Ψ , the combination $\Theta_0(\eta_*) + \Psi(\eta_*)$ is the quantity associated with observed temperature fluctuations.

The gravitational potential $\Phi(\eta_*)$ is related to the value $\Phi(\eta_0)$ at today ($a_0 = 1$), as $\Phi(\eta_0)/\Phi(\eta_*) = D(a_0)$, where D is the growth factor. Then, today's value of Θ_l induced by the SW effect reads

$$\Theta_l^{\text{SW}}(\eta_0) = -\frac{1}{3D(a_0)}\Phi(\eta_0)j_l(k\eta_0), \quad (7.212)$$

where we used $\eta_0 \gg \eta_*$. Since the power spectrum of $\Phi(\eta_0)$ is given by Eq. (7.151), Eq. (7.161) reduces to

$$C_l^{\text{SW}} = \frac{4\pi}{25} \frac{\mathcal{P}_{\mathcal{R}}(k_0)}{k_0^{n_s-1}} \int_0^\infty dk k^{n_s-2} T^2(k) j_l^2(k\eta_0). \quad (7.213)$$

Since $T(k) \simeq 1$ for $k \ll k_{\text{eq}}$, Eq. (7.213) can be integrated to give

$$C_l^{\text{SW}} = \frac{\pi^{3/2}}{25} \frac{\mathcal{P}_{\mathcal{R}}(k_0)}{(k_0\eta_0)^{n_s-1}} \frac{\Gamma[(3-n_s)/2]\Gamma[l+(n_s-1)/2]}{\Gamma[2-n_s/2]\Gamma[l+(5-n_s)/2]}, \quad (7.214)$$

where Γ is the Gamma function. Since the curvature perturbation generated during inflation is close to scale-invariant ($n_s = 1$), Eq. (7.214) reduces to

$$\frac{l(l+1)C_l^{\text{SW}}}{2\pi} = \frac{\mathcal{P}_{\mathcal{R}}(k_0)}{25}. \quad (7.215)$$

In Fig. 7.2, we show the observational data of $\mathcal{D}_l = l(l+1)C_lT_0^2/(2\pi)$ provided by the Planck mission. As predicted by Eq. (7.215), the quantity $l(l+1)C_l/(2\pi)$ is nearly constant for low multipoles ($l \lesssim 20$). The observed value is $l(l+1)C_lT_0^2/(2\pi) \simeq 7 \times 10^{-10} \text{ K}^2$ for $l = 10$, so the amplitude of the primordial power spectrum is known as $\mathcal{P}_{\mathcal{R}}(k_0) \simeq 2 \times 10^{-9}$ (see Eq. (6.196) for the precise bound). Hence the energy scale of inflation can be constrained from the CMB measurements.

The shaded region in Fig. 7.2, characterizes the systematic uncertainty called the cosmic variance. From Eq. (7.156) the quantity C_l is the variance of a_{lm} . There

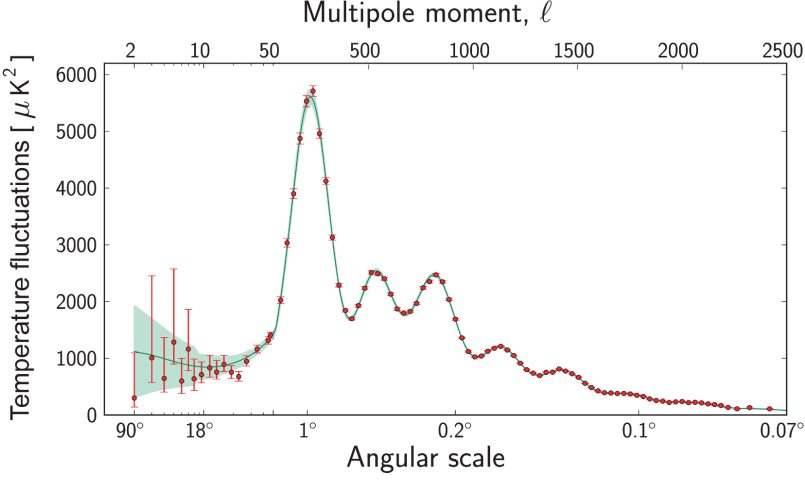


Fig. 7.2. The CMB angular power spectrum observed by the Planck satellite (red points) and the best-fit Λ CDM model (green line). The horizontal and vertical axes correspond to the multipole l (or $\theta = 180^\circ/l$) and the temperature fluctuation $\mathcal{D}_l = l(l+1)C_l T_0^2/(2\pi)$, respectively, with the present temperature $T_0 = 2.725$ K. The error bars contain the contribution from the cosmic variance. Reproduced from Ref. [13].

are $2l+1$ components of integer m for each l . Since the variance of C_l for each l is given by $\Delta C_l^2 = 2C_l^2/(2l+1)$, the uncertainty arising from the cosmic variance gets larger for smaller multipoles ($l \lesssim 10$). On the other hand, small-scale temperature anisotropies are less affected by such uncertainty.

In Fig. 7.2, we also show the theoretical prediction of the angular power spectrum for the best-fit Λ CDM model. For the multipoles l smaller than 10, the quantity $l(l+1)C_l/(2\pi)$ slightly increases toward larger scales. This is attributed to the late-time ISW effect induced by the presence of dark energy as well as to the slightly red-tilted spectrum constrained as Eq. (6.197).

Next, we study the temperature anisotropies on smaller scales ($l \gg 1$). The value of $\Theta_0(k, \eta_*)$ in Eq. (7.210) can be approximately derived by setting $\eta = \eta_*$ in Eq. (7.174). The position of the first acoustic peak estimated by the first line of Eq. (7.174) is given by Eq. (7.181). The spherical Bessel function in the first and second lines of Eq. (7.210) approximately reads $j_l[k(\eta_0 - \eta_*)] \simeq j_l(k\eta_0)$. The function $j_l(x)$ defined by Eq. (7.203) satisfies $j_l(0) = 0$ for $l \geq 1$. As x increases from 0, $j_l(x)$ increases and it has a maximum value at $x = x_1$ (e.g., $x_1 = 3.3$ for $l = 2$). For $x > x_1$, $j_l(x)$ decreases with oscillations. If $l \gg 1$, then $j_l(x)$ is close to 0 in the regime $0 \leq x \ll x_1$ and $j_l(x)$ starts to increase for x close to x_1 . This means that the main contribution to $j_l(k\eta_0)$ comes from $k\eta_0 > x_1$. Since x_1 is close to l for $l \gg 1$, the main contributions to the first and second lines of Eq. (7.210) are the modes

$$k\eta_0 > l. \quad (7.216)$$

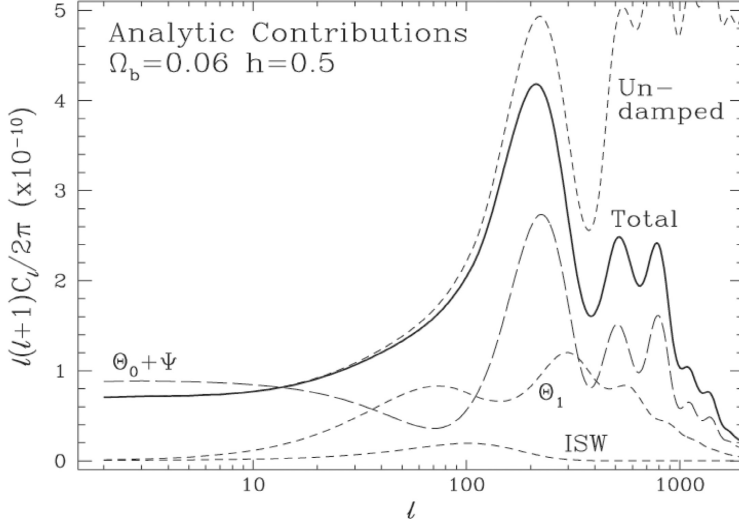


Fig. 7.3. Analytic estimation for the angular power spectrum of temperature anisotropies in the flat CDM model with $\Omega_b^{(0)} = 0.06$, $h = 0.5$, $n_s = 1$, $r = 0$. The three curves in the bottom show the contributions from $\Theta_0 + \Psi$, Θ_1 , and the early ISW effect. The solid and dotted curves are the total angular power spectra with and without the Silk damping, respectively. Reproduced from Ref. [4].

In reality x_1 is slightly larger than l , so the positions of peaks associated with the perturbations $\Theta_0(k, \eta_*) + \Psi(k, \eta_*)$ tend to shift toward smaller l . In addition, the value of C_l defined by Eq. (7.161) is the integral with respect to all k , so this leads to the change of the positions of peaks. In general, the values of l_m corresponding to peaks and troughs are related to l_A in Eq. (7.181), as [14]

$$l_m = l_A(m - \phi_m). \quad (7.217)$$

The peaks and troughs correspond to integers m and half-integers m , with ϕ_m characterizing the deviation of l . The first peak has been constrained to be $l_A \simeq 302$ from WMAP and Planck observations, in which case $\phi_1 \simeq 0.265$ and $l_m \simeq 222$.

In Fig. 7.3, we plot the contribution $\Theta_0 + \Psi$ in the total angular power spectrum for the flat CDM model without dark energy. This is the main contribution to the total power spectrum given in Eq. (7.210). The phase of Θ_1 in Eq. (7.210) is different from that of $\Theta_0 + \Psi$ by the amount $\pi/2$, so if the latter is a trough, the former is a peak. This property can be confirmed in Fig. 7.3. For the multipoles $l \gtrsim 10$ the total amplitude of C_l increases by the presence of Θ_1 , so we cannot ignore the effect of Θ_1 for the correct estimation of C_l .

In Fig. 7.3, the existence of dark energy is not taken into account, so the gravitational potentials Φ and Ψ remain constant from the onset of the matter era to today. In this case the late-time ISW effect does not cause the modification to C_l , but the

early ISW effect that occurs during the transition from the radiation era to the matter era affects C_l . Since this occurs around $\eta = \eta_*$, the modes $l < k\eta_0 \approx k/H_0$, which are the same as Eq. (7.216), are the main sources for the last term of Eq. (7.210). This means that, for larger l , only the perturbations deep inside today's Hubble radius ($k \gg H_0$) contribute to the ISW effect. The quantity characterizing the early ISW effect is the difference between the gravitational potentials at $\eta = \eta_*$ and $\eta = \eta_0$. As we see in Fig. 7.1, the gravitational potential Φ damps earlier for perturbations on smaller scales, so the quantity $\Phi(\eta_*) - \Phi(\eta_0)$ tends to be smaller compared to perturbations on larger scales. Thus, the early ISW effect is important for the multipoles l less than 300.

In the presence of dark energy, the gravitational potential Φ for large-scale perturbations starts to decrease for the redshift $z \lesssim 3$, so this gives rise to the late-time ISW effect. The late-time ISW effect is significant for perturbations with low multipoles ($l \lesssim 10$), reflecting the fact that smaller-scale perturbations are subject to earlier damping. Compared to the CDM model in which Φ stays constant after the onset of the matter era, the existence of dark energy induces the larger amplitude of C_l for $l \lesssim 10$ due to the late-time ISW effect.

The dotted line at the top of Fig. 7.3 does not take into account the effect of Silk damping, so this does not provide the correct estimation of C_l for $l \gtrsim 200$. In Eq. (7.210), we can accommodate the effect of Silk damping by changing

$$(\Theta_0 + \Psi)(k, \eta_*) \rightarrow (\Theta_0 + \Psi)(k, \eta_*)\mathcal{D}(k), \quad (7.218)$$

$$\Theta_1(k, \eta_*) \rightarrow \Theta_1(k, \eta_*)\mathcal{D}(k), \quad (7.219)$$

where

$$\mathcal{D}(k) = - \int_0^{\eta_0} d\eta g(\eta) \exp[-k^2/k_D^2(\eta)]. \quad (7.220)$$

The quantities k_D^{-1} and $g(\eta)$ are defined, respectively, by Eqs. (7.195) and (7.209). The solid curve in Fig. 7.3, which takes into account the effect of Silk damping, can reproduce the fully numerically derived angular power spectrum with the accuracy less than 10% [4].

7.11. Constraints on cosmological parameters

The CMB temperature anisotropies depend on numerous cosmological parameters. From Eq. (7.174), the monopole Θ_0 is related to the sound speed c_s , which depends on the amount of baryons. Let us first discuss how the CMB angular power spectrum is affected by the change of the amount of baryons. The last term on the right hand side of Eq. (7.174) corresponds to the forced terms induced by gravitational potentials. Neglecting the time variations of Ψ and Φ from the asymptotic past

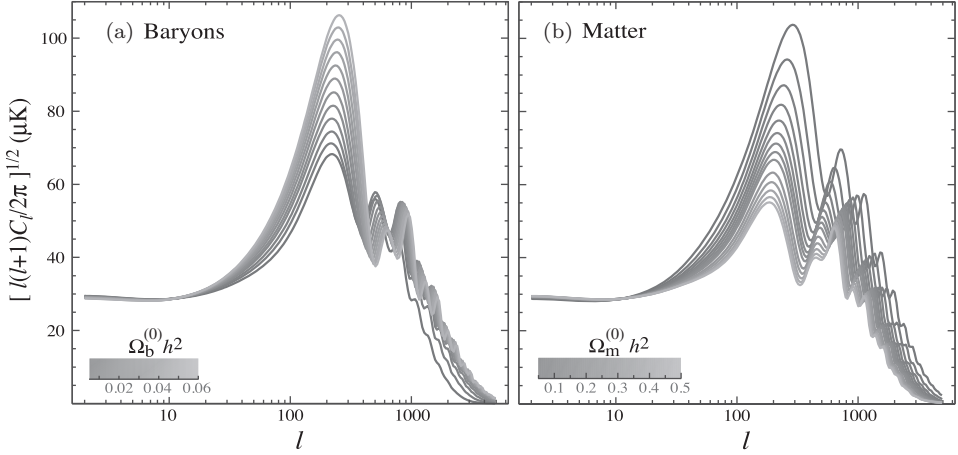


Fig. 7.4. The left and right panels show how the CMB angular power spectrum is modified when the amounts of baryons ($\Omega_b^{(0)}h^2$) and non-relativistic matter ($\Omega_m^{(0)}h^2$) are varied, respectively. Reproduced from Ref. [15].

($\eta = 0$) to $\eta = \eta_*$ and assuming that c_s is constant, Eq. (7.174) reduces to

$$\Theta_0(\eta_*) + \Phi(\eta_*) \approx [\Theta_0(0) + \Phi(0)] \cos(kr_s(\eta_*)) + \frac{\Phi(0) - \Psi(0)}{\sqrt{3}c_s} [1 - \cos(kr_s(\eta_*))]. \quad (7.221)$$

At the peak position characterized by Eq. (7.175), the last term of Eq. (7.221) reads $2[\Phi(0) - \Psi(0)]/(\sqrt{3}c_s)$ for odd n , which increases for larger amount of baryons (i.e., for smaller c_s). This corresponds to the epoch at which the harmonic oscillator shrinks maximally. For even n , the last term of Eq. (7.221) is equivalent to 0 at acoustic peaks, so the amplitude of temperature perturbations is not affected by the change of amount of baryons. In summary, the height of odd-number acoustic peaks increases for larger $\Omega_b^{(0)}$, whereas the even-number acoustic peaks are not affected much (see Fig. 7.4). Since the change of height is sensitive to the amount of baryons, $\Omega_b^{(0)}h^2$ is constrained as Eq. (4.63) from the Planck data.

Let us next consider the case in which $\Omega_m^{(0)}h^2$ is increased while $\Omega_{\text{DE}}^{(0)}$ and $\Omega_{\mathcal{K}}^{(0)}$ are fixed. Since there is the relation $\Omega_m^{(0)} + \Omega_{\text{DE}}^{(0)} + \Omega_{\mathcal{K}}^{(0)} = 1$, we increase h^2 while $\Omega_m^{(0)}$ is fixed. From Eq. (4.80), the redshift z_{eq} tends to be larger for increasing $\Omega_m^{(0)}h^2$, so the amount of radiation at $z = z_*$ gets smaller than that of dark matter. This means that the epoch at which the Universe enters the matter-dominated epoch gets earlier for larger $\Omega_m^{(0)}h^2$, so the damping of gravitational potentials occurs in the earlier epoch. Then, the suppression induced by the early ISW effect works for the modes around the first acoustic peak (see Fig. 7.4). For larger $\Omega_m^{(0)}h^2$, the value of $H(z)$ for $z < z_*$ increases from Eq. (4.78), so the comoving diameter distance $D_A(z_*) = \int_0^{z_*} dz/H(z)$ (for $\mathcal{K} = 0$) to $z = z_*$ gets smaller. Then the visual angle

θ of the CMB map effectively increases, so the CMB power spectrum tends to shift toward smaller l . The Planck CMB data constrained the amount of CDM, as Eq. (4.67).

We also consider the case in which $\Omega_{\mathcal{K}}^{(0)}$ is increased, while $\Omega_{\text{DE}}^{(0)}$ and $\Omega_m^{(0)}h^2$ are fixed. In this case, the quantity $D_A(\eta_*)$ given by Eq. (7.180) increases due to the lensing deformation in the open Universe. The visual angle θ decreases for larger $\Omega_{\mathcal{K}}^{(0)}$, so the power spectrum shifts toward larger l .

If we increase $\Omega_{\text{DE}}^{(0)}$ with $\Omega_{\mathcal{K}}^{(0)}$ and $\Omega_m^{(0)}h^2$ fixed, then the power spectrum shifts toward smaller l due to the decrease of $D_A(\eta_*)$. As we will see in Sec. 8, this property can be used to constrain the property of dark energy. Moreover, the late-time ISW effect induced by dark energy leads to the modification to C_l for large-scale perturbations.

The CMB power spectrum depends on the initial amplitude $\mathcal{P}_{\mathcal{R}}$, the spectral index n_s , and the running spectral index α_s of primordial curvature perturbations generated during inflation. In the early Universe the primordial tensor perturbations are also generated, so the tensor-to-scalar ratio r and the tensor spectral index n_t are the observable quantities. As we explained in Sec. 6.8, the inflationary paradigm predicts r much smaller than 1. The tensor perturbations start to decay after the horizon reentry, so they contribute to the large-scale temperature anisotropies with $l < 100$. The Planck observations put the upper bound on r , as Eq. (6.198). The future measurements of CMB B-modes will offer the possibility for placing tight bounds on r .

There are other effects that modify the CMB power spectrum. One of them is the reionization of the Universe. After compact objects start to be formed in the matter era, the emission of electromagnetic waves from them leads to the ionization of neutral hydrogen. The CMB photons are partially scattered by this reionization, so the CMB power spectrum is subject to modifications. The function $g(\eta)$ defined by Eq. (7.209) obeys $\int_0^{\eta_0} g(\eta)d\eta = 1$, so the probability of photons being scattered by electrons per time interval $d\eta$ is $g(\eta)d\eta = -e^{-\tau}d\tau$. Integrating this relation from the moment of reionization ($\tau = \tau_{\text{ion}}$) to the present ($\tau = 0$), the scattering probability of photons is given by $1 - e^{-\tau_{\text{ion}}}$. Since the probability that photons are not scattered is $e^{-\tau_{\text{ion}}}$, the temperature $T(1 + \Theta)$ of CMB photons is multiplied by the suppression factor $e^{-\tau_{\text{ion}}}$. Adding the contribution of the temperature $T(1 - e^{-\tau_{\text{ion}}})$ of scattered photons, the temperature of CMB photons due to the reionization can be estimated as $T(1 + \Theta e^{-\tau_{\text{ion}}})$. This means that the temperature perturbation Θ is suppressed by the factor $e^{-\tau_{\text{ion}}}$. This suppression works for perturbations inside the Hubble radius at the reionization epoch. The Planck constraint on the optical depth is given by [13]

$$\tau_{\text{ion}} = 0.089_{-0.014}^{+0.012} \quad (68\% \text{ CL}). \quad (7.222)$$

This corresponds to the redshift around $z_{\text{ion}} = 10$.

The CMB spectrum is also subject to distortions due to the so-called Sunyaev-Zel'dovich (SZ) effect [16] in which photons acquire the energy from high-temperature electrons in galaxies through the inverse Compton scattering. Since the SZ effect hardly depends on the redshift z , its detection at high z is possible. However, the amplitude A_{SZ} of the SZ effect is small, so its observations is generally not so easy.

Numerical techniques have been developed to constrain cosmological parameters from the observational data of CMB temperature anisotropies. Seljak and Zaldarriaga developed a numerical code called the CMBFAST for computing the CMB power spectrum efficiently in terms of the line-of-sight integral [17]. Lewis and Challinor made a Monte Carlo simulation code called CosmoMC by improving the CMBFAST [18]. The latter code can constrain cosmological parameters best fitted to the CMB and other observational data.¹ The following cosmological parameters are given in the CosmoMC code as a default:

$$\Omega_b^{(0)} h^2, \Omega_c^{(0)} h^2, \theta_A, \tau_{\text{ion}}, \Omega_{\mathcal{K}}^{(0)}, f_\nu, w_{\text{DE}}, n_s, n_t, \alpha_s, \mathcal{P}_{\mathcal{R}}(k_0), r, A_{\text{SZ}}, \quad (7.223)$$

where $\theta_A = \pi/l_A$, and f_ν is the ratio of massive neutrinos relative to dark matter. The quantities H_0 and $\Omega_{\text{DE}}^{(0)}$ are related to the parameters given in Eq. (7.223). The solid curve in Fig. 7.2 corresponds to the best-fit Λ CDM model ($w_{\text{DE}} = -1$) derived by the likelihood analysis using the CosmoMC. This shows good agreement with the Planck CMB data especially for $l \gtrsim 50$ (in which regime the cosmic variance is small). The Planck satellite precisely measured the CMB temperature anisotropies up to the multipole $l \simeq 2500$. This allowed us to put tight constraints on numerous cosmological parameters mentioned above.

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¹The numerical code can be downloaded from <http://cosmologist.info/cosmomc/>.

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Chapter 8

Observational Probes for Dark Energy from CMB, Galaxy Clusterings, BAO, Weak Lensing

In Sec. 5.3, we explained how the late-time cosmic acceleration was discovered from the SN Ia measurements. The discussions given in Sec. 5.3 were based on observational constraints on dark energy at the background level. In this section, we study observational signatures of dark energy extracted from the information of cosmological perturbations. We discuss how the property of dark energy can be constrained from the measurements of CMB, galaxy clusterings, redshift-space distortions, and weak lensing.

8.1. CMB

In Chap. 7, we discussed how the CMB temperature anisotropies are related with numerous cosmological parameters. The existence of dark energy affects the CMB power spectrum at least in two ways. First, the change of the angular diameter distance from the last scattering surface to today leads to the shift of CMB acoustic peaks. Second, the variation of gravitational potentials induced by the presence of dark energy gives rise to the late-time ISW effect. The latter is limited on large-scale temperature anisotropies, where the observational data are affected by the cosmic variance. The first effect is usually more important to constrain the property of dark energy.

The multipole l_A given by Eq. (7.176), i.e.,

$$l_A = \pi \frac{D_A(z_*)}{r_s(z_*)}, \quad (8.1)$$

characterizes the angular scale of the sound horizon at CMB last scattering (redshift z_*). This quantifies the ratio between the comoving angular diameter distance $D_A(z_*)$ to the decoupling epoch and the sound horizon $r_s(z_*)$. The multipole

l_A can be expressed as Eq. (7.181) by using the CMB shift parameter $\mathcal{R}_{\text{CMB}}$ defined by Eq. (7.180). From Eq. (7.179), $\mathcal{R}_{\text{CMB}}$ is related to another distance ratio $D_A(z_*)/H_0^{-1}$, as

$$\mathcal{R}_{\text{CMB}} = \sqrt{\Omega_m^{(0)}} \frac{D_A(z_*)}{H_0^{-1}}. \quad (8.2)$$

The fitting formula of the redshift z_* is given by Eq. (7.15), which depends on the quantities $\omega_b = \Omega_b^{(0)} h^2$ and $\omega_m = \Omega_m^{(0)} h^2$.

To understand how the information of dark energy can be extracted from the CMB shift parameter, we consider the flat FLRW background with $\mathcal{K} = 0$. In this case, Eq. (7.180) reduces to

$$\mathcal{R}_{\text{CMB}} = \sqrt{\Omega_m^{(0)}} \int_0^{z_*} \frac{dz}{E(z)}. \quad (8.3)$$

The CMB shift parameter $\mathcal{R}_{\text{CMB}}$ contains the integral of the quantity $H_0/H(z)$ from $z = 0$ to $z = z_*$, so it can be used to constrain the property of dark energy. If we consider a constant dark energy equation of state w_{DE} , the normalized Hubble parameter $E(z) = H(z)/H_0$ is given by

$$E(z) = [\Omega_r^{(0)}(1+z)^4 + \Omega_m^{(0)}(1+z)^3 + \Omega_{\text{DE}}^{(0)}(1+z)^{3(1+w_{\text{DE}})}]^{1/2}, \quad (8.4)$$

where we used Eq. (4.78).

In Fig. 8.1, we plot $\mathcal{R}_{\text{CMB}}$ versus $\Omega_m^{(0)}$ for three different values of w_{DE} with $\Omega_r^{(0)} = 8.5 \times 10^{-5}$ and $z_* = 1090$. For given $\Omega_m^{(0)}$, the CMB shift parameter tends to be larger for smaller w_{DE} . Assuming a standard FLRW cosmology with adiabatic perturbations, the CMB shift parameter constrained from the Planck 2015 data (temperature data and low l polarization data) is given by [1]

$$\mathcal{R}_{\text{CMB}} = 1.7488 \pm 0.0074, \quad (8.5)$$

at 68% CL. This bound is plotted as a shaded region in Fig. 8.1. For the cosmological constant ($w_{\text{DE}} = -1$), the matter density parameter is observationally constrained to be around $\Omega_m^{(0)} = 0.3$. This is consistent with the bounds on $\Omega_m^{(0)}$ derived from the SN Ia data. From Fig. 8.1, we find that, for increasing w_{DE} , the values of $\Omega_m^{(0)}$ constrained from the Planck bound of $\mathcal{R}_{\text{CMB}}$ tend to be larger.

The CMB shift parameter (8.3), which depends on $\Omega_m^{(0)}$ and z_* , is not sufficient to extract the full likelihood information to place CMB constraints on dark energy. It is possible to compress a large part of the full CMB likelihood information in terms of four parameters: (1) the shift parameter $\mathcal{R}_{\text{CMB}}$, (2) the multipole l_A , (3) the baryon density $\omega_b = \Omega_b^{(0)} h^2$, and (4) the scalar spectral index n_s .

Since l_A determines the average acoustic peak structure, models with the same value of $\mathcal{R}_{\text{CMB}}$ but with different values of l_A give rise to different CMB angular power spectra [2, 3]. Models with the same value of l_A but with different values of $\mathcal{R}_{\text{CMB}}$ have the similar acoustic peak structure, but the overall amplitude of peaks differs due to the difference in $\mathcal{R}_{\text{CMB}}$. Hence we need to use both $\mathcal{R}_{\text{CMB}}$

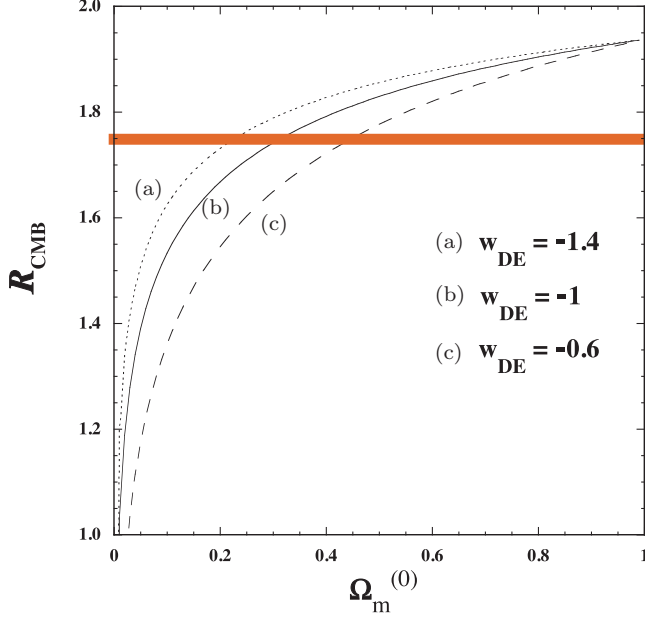


Fig. 8.1. The CMB shift parameter $\mathcal{R}_{\text{CMB}}$ versus $\Omega_m^{(0)}$ for three different values of w_{DE} with $\Omega_r^{(0)} = 8.5 \times 10^{-5}$ and $z_* = 1090$. We also plot the Planck observational bound $\mathcal{R}_{\text{CMB}} = 1.7488 \pm 0.0074$ as a shaded region. For larger w_{DE} , the values of $\Omega_m^{(0)}$ constrained from the Planck bound of $\mathcal{R}_{\text{CMB}}$ get larger.

and l_A besides ω_b and n_s to place constraints on dark energy parameters like $w_{\text{DE}}^{(0)}$ and $\Omega_{\text{DE}}^{(0)}$. We can use z_* instead of ω_b , but the latter is more appropriate in the cosmological Monte-Carlo simulation like CosmoMC (since ω_b is a base parameter in the code).

From the Planck data of temperature and low- l polarization data the posterior distribution of $\mathcal{R}_{\text{CMB}}, l_A, \omega_b, n_s$ is approximately Gaussian, with marginalized mean values and variances [1]:

$$\langle \mathcal{R}_{\text{CMB}} \rangle = 1.7488, \quad \sigma(\mathcal{R}_{\text{CMB}}) = 0.0074, \quad (8.6)$$

$$\langle l_A \rangle = 301.76, \quad \sigma(l_A) = 0.14, \quad (8.7)$$

$$\langle \omega_b \rangle = 0.02228, \quad \sigma(\omega_b) = 0.00023, \quad (8.8)$$

$$\langle n_s \rangle = 0.9660, \quad \sigma(n_s) = 0.0061. \quad (8.9)$$

The normalized covariance matrix of $(\mathcal{R}_{\text{CMB}}, l_A, \omega_b, n_s)$ derived from a Monte Carlo Markov chain approach is

$$\mathcal{D}_{ij} = \begin{pmatrix} 1.00 & 0.54 & -0.63 & -0.86 \\ 0.54 & 1.00 & -0.43 & -0.48 \\ -0.63 & -0.43 & 1.00 & 0.58 \\ -0.86 & -0.48 & 0.58 & 1.00 \end{pmatrix}. \quad (8.10)$$

The covariance matrix reads

$$\mathcal{C}_{ij} = \sigma(p_i) \sigma(p_j) \mathcal{D}_{ij}, \quad (8.11)$$

with the four parameters $p_1 = \mathcal{R}_{\text{CMB}}, p_2 = l_A, p_3 = \omega_b, p_4 = n_s$. The χ^2 of a given model can be computed by the formula

$$\chi_{\text{CMB}}^2 = \Delta p_i \mathcal{C}_{ij}^{-1} \Delta p_j, \quad \Delta p_i = p_i - p_i^{\text{data}}, \quad (8.12)$$

where p_i^{data} are the mean values given by Eqs. (8.6)–(8.9), and $\mathcal{C}_{ij}^{-1}$ is the inverse of the covariance matrix $\mathcal{C}_{ij}$.

We recall that the χ^2 in SN Ia observations can be computed from Eq. (5.19). The model best fitted to SN Ia and CMB measurements is the case in which

$$\chi^2 = \chi_{\text{SN Ia}}^2 + \chi_{\text{CMB}}^2 \quad (8.13)$$

is minimized. For the constant w_{DE} model, the computation of χ^2 allows one to put constraints on w_{DE} and $\Omega_{\text{DE}}^{(0)}$.

In Fig. 8.2, we show observational bounds on w_{DE} and $\Omega_m^{(0)}$ derived from the joint data analysis of SN Ia and CMB. The allowed parameter space from the CMB data is almost orthogonal to that from the SN Ia data. The region constrained from the CMB data shown in Fig. 8.2 is consistent with the discussion of using $\mathcal{R}_{\text{CMB}}$ already explained: the observationally allowed values of w_{DE} increase for larger $\Omega_m^{(0)}$.

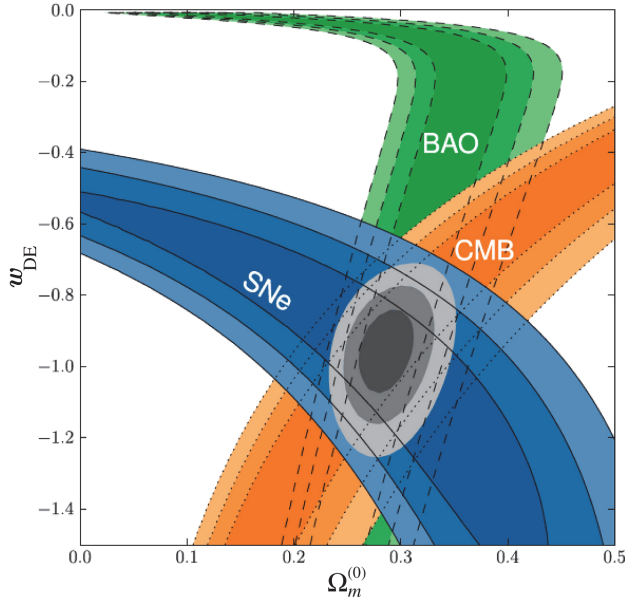


Fig. 8.2. The 68.3%, 95.4%, and 99.7% confidence regions in the $(\Omega_m^{(0)}, w_{\text{DE}})$ plane constrained from SN Ia, CMB (WMAP), and BAO data. The dark energy equation of state w_{DE} is assumed to be constant. The confidence regions include both statistical and systematic uncertainties. Reproduced from Ref. [4].

Even if the CMB data alone do not provide strong constraints on w_{DE} and $\Omega_m^{(0)}$, the joint data analysis of CMB and SN Ia give tighter bounds on these parameters. In Fig. 8.2, we observe that the dark energy equation of state needs to be in the range $-1.3 < w_{\text{DE}} < -0.8$ at 95% CL for the model with constant w_{DE} .

The likelihood values (8.6)–(8.9) of $\mathcal{R}_{\text{CMB}}, l_A, \omega_b, n_s$ and the normalized covariance matrix (8.10) were derived for the constant w_{DE} model, but it was confirmed that the same compressed likelihood can be also used for “smooth dark energy models” in which the variation of w_{DE} is not rapid [1–3]. This includes the CPL parametrization with two parameters w_0 and w_a given by Eq. (5.23). The joint observational constraints on the model parameters w_0 and w_a derived from CMB and SN Ia (JLA) data are shown in Fig. 5.4. Since there is one more free parameter w_a in the CPL parametrization relative to the constant w_{DE} model, the allowed region of w_0 in the former is wider than that in the latter.

The compressed likelihood explained above is convenient in that the information about dark energy can be extracted without explicitly solving perturbed Boltzmann and Einstein equations. It can be applied to a wide class of smooth dark energy models in the framework of GR. In modified gravitational theories, however, the effective gravitational coupling with non-relativistic matter is generally modified from that of GR. As we will see in Sec. 15.6, a numerical code called EFTCAMB was developed to place observational constraints on modified gravity models.

8.2. Gravitational instabilities

As we will see in Sec. 8.6, the property of dark energy can be further constrained from the data of baryon acoustic oscillations (BAO). Since this is related to two-point correlation functions of galaxy clusterings, we first review the basics of structure formations in this section. In Sec. 8.3, we derive the matter power spectrum in redshift space and in Sec. 8.4, we discuss how the growth rate of matter perturbations can be constrained from the measurements of redshift space distortions. In Sec. 8.6, we study how the BAO data place constraints on the property of dark energy.

In Sec. 6.5, we derived the perturbation equations in the presence of a fluid or a scalar field and discussed the evolution of matter perturbations δ_m in Sec. 7.6. In the framework of GR, the matter perturbation whose wavelength is smaller than the Hubble radius grows in proportion to the scale factor a during the matter era, see Eq. (7.142). In what follows, we study in more detail how CDM and baryon perturbations grow due to the gravitational instability.

Let us first consider a fluid without having the anisotropic stress Π for the perturbed metric (7.17) in the Newtonian gauge. We define the two quantities associated with the density perturbation $\delta\rho$ and the velocity potential v , as

$$\delta = \frac{\delta\rho}{\rho}, \quad \theta = \frac{\nabla^2 v}{\mathcal{H}}, \quad (8.14)$$

where $\mathcal{H} = aH$. On using the equation of state $w = P/\rho$ and the sound speed c_s defined by Eq. (6.127), the perturbed equations of motion (6.105) and (6.107) in Fourier space reduce, respectively, to

$$\delta' + 3\mathcal{H}(c_s^2 - w)\delta = -(1 + w)(3\Phi' + \mathcal{H}\theta), \quad (8.15)$$

$$\theta' + \left[\mathcal{H}(1 - 3w) + \frac{\mathcal{H}'}{\mathcal{H}} + \frac{w'}{1 + w} \right] \theta = \frac{k^2}{\mathcal{H}} \left(\frac{c_s^2}{1 + w} \delta + \Psi \right), \quad (8.16)$$

where a prime represents a derivative with respect to η . If the dominant contribution to the energy density of the Universe comes from the single fluid, the Poisson equation (6.130) reads

$$k^2\Phi = 4\pi G a^2 \rho \hat{\delta}, \quad (8.17)$$

where $\hat{\delta}$ is a gauge-invariant quantity defined by Eq. (6.129), i.e.,

$$\hat{\delta} = \delta + 3 \left(\frac{\mathcal{H}}{k} \right)^2 (1 + w)\theta. \quad (8.18)$$

The gauge-invariant sound speed $\hat{c}_s$ is defined by Eq. (6.131), which is related to c_s as

$$c_s^2 = \hat{c}_s^2 + 3 \left(\frac{\mathcal{H}}{k} \right)^2 (1 + w)(\hat{c}_s^2 - c_a^2) \frac{\theta}{\delta}, \quad (8.19)$$

where c_a is the adiabatic sound speed given by Eq. (6.126).

We focus on the perturbations whose wavelengths are much smaller than the Hubble radius ($k \gg \mathcal{H}$). In this case we have $\hat{\delta} \simeq \delta$ and $\hat{c}_s^2 \simeq c_s^2$, so we omit the hat in the following discussion. We consider the case in which the Universe is dominated by non-relativistic matter characterized by $w \simeq 0$ and $c_s^2 \ll 1$. Since $3\mathcal{H}^2 \simeq 8\pi G a^2 \rho$ in this case, we obtain $|\Phi| \simeq 3\mathcal{H}^2 |\delta| / (2k^2) \ll |\delta|$ from Eq. (8.17). Then the term Φ' on the right hand side of Eq. (8.15) can be neglected, so that

$$\delta' \simeq -\mathcal{H}\theta. \quad (8.20)$$

Equation (8.16) reduces to

$$\theta' + \left(\mathcal{H} + \frac{\mathcal{H}'}{\mathcal{H}} \right) \theta = \frac{k^2}{\mathcal{H}} (c_s^2 \delta + \Psi). \quad (8.21)$$

Taking the η derivative of Eq. (8.20) and employing Eqs. (8.17) and (8.21), it follows that

$$\delta'' + \mathcal{H}\delta' + (c_s^2 k^2 - 4\pi G a^2 \rho) \delta = 0, \quad (8.22)$$

where we used the relation $\Psi \simeq -\Phi$ after the end of the radiation era. The term $c_s^2 k^2$ corresponds to the pressure term associated with the propagation of the sound speed, which prevents the growth of δ . The term $-4\pi G a^2 \rho$ leads to the enhancement of δ due to the gravitational instability. The growth of matter perturbations occurs

under the condition $k < a\sqrt{4\pi G\rho}/c_s \equiv k_J$. The physical wavelength corresponding to k_J is given by

$$\lambda_J = \frac{2\pi a}{k_J} = c_s \sqrt{\frac{\pi}{G\rho}}, \quad (8.23)$$

which is known as the Jeans length. The perturbations with the wavelength λ larger than λ_J exhibit growth, whereas, for $\lambda < \lambda_J$, the pressure term prevents the gravitational attraction. On using the relation $3H^2 = 8\pi G\rho$, we can estimate the Jeans length, as $\lambda_J \approx (c_s/c)(cH^{-1})$. If c_s is much smaller than the speed of light c , λ_J is much smaller than the Hubble radius cH^{-1} . In this case, the growth of perturbations occurs on scales relevant to large-scale structures of the Universe.

For the perfect fluid with constant w we have $c_s^2 = c_a^2 = w$, so that $c_s^2 \simeq 0$ for non-relativistic matter. Since the Jeans length is very small during the matter era, the structure formation occurs on most of scales. During the radiation era the sound speed of the photon–baryon fluid is given by (7.163), i.e., $c_s \approx 1/\sqrt{3}$, so the Jeans length is of the same order as the Hubble radius. In the latter case, the baryon perturbations do not grow for most of the modes inside the Hubble radius.

Let us consider the evolution of CDM and baryon perturbations during the transient epoch from the radiation era to the matter era. Then, the system is described by three fluids including radiation. For the modes $k \gg \mathcal{H}$, the Poisson equation (7.107) reduces to

$$k^2\Phi \simeq 4\pi Ga^2(\rho_c\delta_c + \rho_b\delta_b + 4\rho_r\Theta_{r,0}). \quad (8.24)$$

In the following, we consider the case in which the radiation perturbation can be neglected relative to the perturbations of non-relativistic matter ($|4\rho_r\Theta_{r,0}| \ll |\rho_c\delta_c + \rho_b\delta_b|$). Setting $c_s = 0$ for CDM and baryon perturbations and employing Eqs. (8.20), (8.21) and (8.24) for each perturbation, it follows that

$$\delta_c'' + \mathcal{H}\delta_c' - 4\pi Ga^2(\rho_c\delta_c + \rho_b\delta_b) = 0, \quad (8.25)$$

$$\delta_b'' + \mathcal{H}\delta_b' - 4\pi Ga^2(\rho_c\delta_c + \rho_b\delta_b) = 0. \quad (8.26)$$

Since $|\rho_c\delta_c| \gg |\rho_b\delta_b|$, neglecting the contribution of baryons in Eq. (8.25) leads to the differential equation of CDM perturbations alone. As in the discussion of Sec. 7.6, we define the dimensionless quantity $y = a/a_{\text{eq}} = \rho_c/\rho_r$ and use the background equations $3H^2 = 8\pi G(\rho_c + \rho_r)$ and $\dot{H} = -4\pi G(\rho_c + 4\rho_r/3)$. Then, Eq. (8.25) approximately reduces to

$$\frac{d^2\delta_c}{dy^2} + \frac{3y+2}{2y(y+1)} \frac{d\delta_c}{dy} - \frac{3}{2y(y+1)} \delta_c \simeq 0. \quad (8.27)$$

The solution to this equation is given by

$$\delta_c = C_1 \left(1 + \frac{3}{2}y\right) + C_2 \left[\left(1 + \frac{3}{2}y\right) \ln \frac{\sqrt{y+1}+1}{\sqrt{y+1}-1} - 3\sqrt{y+1} \right], \quad (8.28)$$

where C_1 and C_2 are integration constants. The second contribution to the right hand side of Eq. (8.28) decreases with the increase of y . Hence the growing mode is given by $\delta_c \propto 1 + (3/2)(a/a_{\text{eq}})$. For $a \ll a_{\text{eq}}$, the CDM perturbation δ_c hardly grows, whereas, for $a \gg a_{\text{eq}}$, it grows as $\delta_c \propto a \propto t^{2/3}$.

For baryons, Eq. (8.26) reduces to

$$\delta_b'' + \mathcal{H}\delta_b' \simeq 4\pi G a^2 \rho_c \delta_c. \quad (8.29)$$

Then, the baryon perturbation is enhanced due to the force term induced by the CDM perturbation. The force term in Eq. (8.29) originates from the gravitational potential generated mainly by CDM. The CDM perturbation starts to grow after the Universe enters the matter-dominated epoch, whereas the growth of baryon perturbations occurs after the CMB decoupling epoch (after which the coupling between baryons and photons becomes weak) to catch up with CDM perturbations.

After the Universe enters the epoch of late-time cosmic acceleration, the evolution of matter perturbations δ_m is subject to change. Taking into account the dark energy perturbation δ_{DE} , the matter perturbations obeys

$$\delta_m'' + \mathcal{H}\delta_m' - 4\pi G a^2 (\rho_m \delta_m + \rho_{\text{DE}} \delta_{\text{DE}}) = 0. \quad (8.30)$$

If the origin of dark energy is the cosmological constant ($w_{\text{DE}} = -1$), we have that $\delta_{\text{DE}} = 0$. In other cases ($w_{\text{DE}} \neq -1$), the dark energy perturbation does not necessarily vanish, whose evolution is generally different depending on the values of w_{DE} and $\hat{c}_s^2$. For example, a canonical scalar field corresponds to $\hat{c}_s^2 = 1$, so δ_{DE} hardly grows due to the presence of pressure. For the models in which $\hat{c}_s^2$ is much smaller than 1, the dark energy perturbation can grow, but as long as w_{DE} is close to -1 , the contribution to the right hand side of Eq. (8.30) from δ_{DE} is generally small [5].

Using the relation $\Omega_m = 8\pi G \rho_m / (3H^2)$ and writing Eq. (8.30) in terms of the derivative with respect to $\mathcal{N} = \ln a$ under the approximation $|\rho_{\text{DE}} \delta_{\text{DE}}| \ll |\rho_m \delta_m|$, we obtain the same equation as Eq. (7.141). From this equation, it is clear that the growth rate of δ_m gets smaller after the cosmic acceleration sets in due to the decrease of Ω_m from 1.

8.3. Matter power spectrum

For non-relativistic matter where $\hat{c}_s^2 k^2$ is much smaller than $4\pi G a^2 \rho$ in Eq. (8.22), the growth of matter perturbations is independent of scales for the modes deep inside the Hubble radius. As we showed in Sec. 7.6, the epoch at which the perturbations enter the Hubble radius depends on their wavelengths. As a result, the gravitational potential Φ has the k dependence, whose property is characterized by the transfer function $T(k)$. The BBKS transfer function (7.148) is close to 1 for $k \ll k_{\text{eq}}$, but for $k \gg k_{\text{eq}}$ it has the dependence $T(k) \propto (\ln k)/k^2$ due to the damping of Φ during the radiation era.

From Eq. (6.130), today's value of $\hat{\delta}_m$ in Fourier space reads

$$\hat{\delta}_m(a_0) = \frac{2}{3\Omega_m^{(0)}} \left(\frac{k}{H_0} \right)^2 \Phi(a_0), \quad (8.31)$$

where we employed the approximation that the dominant contribution to $\hat{\delta}$ comes from non-relativistic matter perturbations, i.e., $\hat{\delta} \simeq \hat{\delta}_m$. The power spectrum $P_\Phi(a_0)$ of the gravitational potential is given by Eq. (7.151), which contains the primordial power spectrum $\mathcal{P}_\mathcal{R}(k_0)$ of curvature perturbations, the scalar spectral index n_s , and the transfer function $T(k)$. From Eqs. (7.151) and (8.31), today's power spectrum of matter perturbations $P_{\delta_m}(k, a_0) = \langle |\hat{\delta}_m(k, a_0)|^2 \rangle$ can be expressed as

$$P_{\delta_m}(k, a_0) = \frac{8\pi^2}{25} \frac{\mathcal{P}_\mathcal{R}(k_0)}{(\Omega_m^{(0)})^2} D^2(a_0) H_0^{-3} \frac{k_0}{H_0} \left(\frac{k}{k_0} \right)^{n_s} T^2(k). \quad (8.32)$$

From the observed CMB temperature anisotropies, $\mathcal{P}_\mathcal{R}(k_0)$ is constrained as Eq. (6.196) at the pivot wavenumber $k_0 = 0.002 \text{ Mpc}^{-1}$. In the CDM model without dark energy, Φ is constant after the onset of the matter era, in which case $D(a_0) = 1$. In the Λ CDM model, Φ decreases during the dark-energy dominated epoch, so $D(a_0)$ is smaller than 1, e.g., $D(a_0) = 0.78$ for $\Omega_m^{(0)} = 0.31$.

For $k \ll k_{\text{eq}}$ the power spectrum (8.32) has the scale dependence $P_{\delta_m}(k, a_0) \propto k^{n_s}$ (with n_s close to 1), which increases for larger k . For $k \gg k_{\text{eq}}$, it has the dependence $P_{\delta_m}(k, a_0) \propto k^{n_s-4} (\ln k)^2$, which decreases for larger k . $P_{\delta_m}(k, a_0)$ has a peak around $k = k_{\text{eq}}$. Since k_{eq} is dependent on $\Omega_m^{(0)}$ from Eq. (7.128), the peak position of $P_{\delta_m}(k, a_0)$ changes depending on the values of $\Omega_m^{(0)}$.

In Fig. 8.3, we plot the matter power spectra computed from Eq. (8.32) in two different cases: (a) the Λ CDM model with $\Omega_m^{(0)} = 0.31$, $D(a_0) = 0.78$, and (b) the CDM model with $\Omega_m^{(0)} = 1$, $D(a_0) = 1$. In the CDM model, $P_{\delta_m}(k, a_0)$ has a peak around $k = 0.07 h \text{ Mpc}^{-1}$, whereas in the Λ CDM model the peak position shifts toward larger scales. This difference of peak positions allows one to place constraints on the amount of dark energy. On small scales characterized by $k > 0.09 h \text{ Mpc}^{-1}$, non-linear effects like the interaction between perturbations with different wavenumbers lead to the modification to the linear power spectrum plotted in Fig. 8.3. In order to take into account such non-linear effects properly, we need to consider gravitational interactions between N particles and study how the particles cluster in the expanding Universe (which is called the N -body simulation) [7].

We relate the galaxy power spectrum P_{δ_g} to the matter power spectrum P_{δ_m} , as

$$P_{\delta_g} = b^2 P_{\delta_m}, \quad (8.33)$$

where the factor b is called a bias. Since the galaxy formation is a non-linear process, the bias factor may depend on scales. Whether the bias is scale-dependent or not has not been completely clarified yet, but the linear bias characterized by constant b is at least a reasonable assumption in the linear regime of the matter power spectrum.

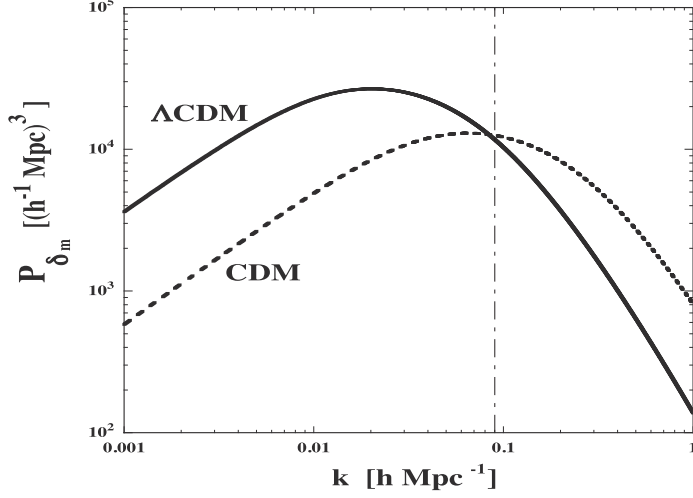


Fig. 8.3. Today's matter power spectra in two cases: (a) the Λ CDM model with $\Omega_m^{(0)} = 0.31$ and $D(a_0) = 0.78$ (solid line), and (b) the CDM model with $\Omega_m^{(0)} = 1$ and $D(a_0) = 1$ (dotted line). We choose the model parameters $h = 0.68$, $\mathcal{P}_{\mathcal{R}}(k_0) = 2.2 \times 10^{-9}$, $n_s = 0.96$ at the pivot wavenumber $k_0 = 0.002 \text{ Mpc}^{-1}$. The dot-dashed vertical line shows the border around which non-linear effects become important ($k > 0.09 h \text{ Mpc}^{-1}$).

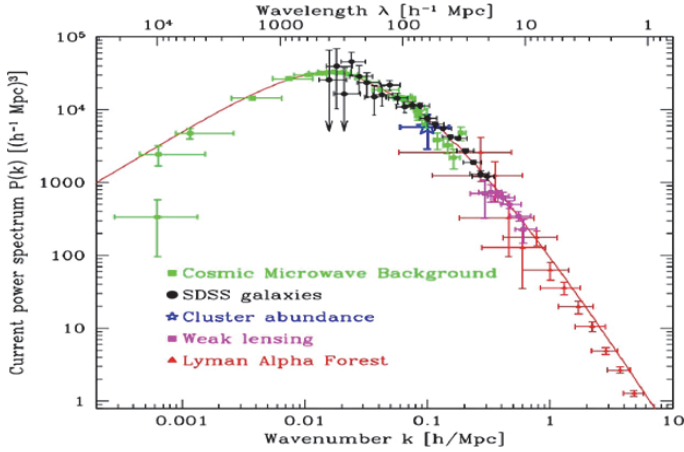


Fig. 8.4. Today's matter power spectrum constrained from the SDSS galaxy surveys with the linear bias $b = 1.3$. The solid curve is the prediction of the Λ CDM model with the model parameters $\Omega_m^{(0)} = 0.3$, $h = 0.7$, and $n_s = 1$. We also show the data extracted from the measurements of CMB, cluster abundance, weak lensing, and Lyman Alpha Forest. Reproduced from Ref. [6].

In Fig. 8.4, we show observational data of today's matter power spectrum constrained from the SDSS galaxy survey and other measurements under the assumption of the linear bias [8]. The observational data are consistent with the theoretical prediction of the Λ CDM model with $\Omega_m^{(0)} = 0.3$ and $n_s = 1$. The matter

power spectrum with the peak around $k = 0.02 h \text{ Mpc}^{-1}$ in the ΛCDM model (as shown in Fig. 8.3) is also compatible with other observational data like CMB. The CDM model without dark energy is disfavored from the galaxy power spectrum with the linear bias. We also note that the nearly scale-invariant primordial power spectrum ($n_s \simeq 1$) predicted by the inflationary paradigm is consistent with numerous observational data plotted in Fig. 8.4.

8.4. Redshift-space distortions

There are two-dimensional and three-dimensional surveys for observing the distribution of galaxies. In the two-dimensional survey, the distance to galaxies is not measured, but we make a map for the distribution of galaxies on the celestial sphere. In the three-dimensional case, we can extract the information about the distance of galaxies by measuring the redshift z from the galaxy distribution. In particular, the latter survey allows one to constrain the growth rate of matter perturbations by measuring galaxy distributions with many different redshifts z .

In three-dimensional galaxy surveys, the observed redshift z is generally different from the corresponding value $\hat{z}$ in the homogenous Universe due to the peculiar velocity of galaxies. Then, the observed power spectrum measured in the redshift space is subject to distortions. We first derive the relation between z and $\hat{z}$. For the perturbed metric (7.17) in the Newtonian gauge, the four-velocity of a galaxy can be expressed as $u_\mu = a(-1 - \Psi, v_{|i})$, where v is the scalar velocity potential. We ignore the contribution to the peculiar velocity from the intrinsic vector mode.

Taking the x -axis from the observer (located at the origin O) to the galaxy and using the spatial unit vector $n^i = (-1, 0, 0)$ pointing from the galaxy to the observer, the four-momentum $P^\mu = (P^0, P^i)$ of a photon emitted from the galaxy to the observer is given by Eq. (7.22) and Eq. (7.23) with $p = E$. If the galaxy has the four-velocity u_μ , the photon frequency yields $\nu = -u_\mu P^\mu$. Neglecting the contribution of the gravitational potential, it follows that

$$\nu = E(1 - n^i v_{|i}). \quad (8.34)$$

Similarly, the photon energy when the observer is moving with the velocity $v_{|i0}$ reads $\nu_0 = E_0(1 - n^i v_{|i0})$. The redshifts z and $\hat{z}$ with and without the peculiar velocity are given, respectively, by $1 + z = \nu/\nu_0$ and $1 + \hat{z} = E/E_0$. Neglecting the second-order terms of perturbations and using the relation $1 + \hat{z} = 1/a$ (with the normalization $a_0 = 1$ today), we obtain

$$z = \hat{z} + \frac{1}{a}(v_x - v_{x0}), \quad (8.35)$$

where $v_x \equiv -n^i v_{|i}$ and $v_{x0} \equiv -n^i v_{|i0}$ are the x components of peculiar velocities of the galaxy and the observer, respectively. From Eq. (8.35), the difference between v_x and v_{x0} leads to the redshift difference $\Delta z = (v_x - v_{x0})/a$.

From Eq. (4.8), the coming distance s in the redshift space is given by

$$s = \int_0^z \frac{dz}{H(z)} \simeq x + \frac{\Delta z}{H(z)} = x + \frac{v_x - v_{x0}}{aH}, \quad (8.36)$$

where we have set $c = 1$. Here, $x = \int_0^z dz/H(z)$ is the comoving distance in real space. If the galaxy number densities in infinitesimal volumes dV_s (redshift space) and dV_x (real space) are given, respectively, by n_s and n_x , then there is the relation $n_s dV_s = n_x dV_x$. The Jacobian associated with the transformation from real space to redshift space is

$$J = \left| \frac{\partial s}{\partial x} \right| \simeq 1 + \frac{1}{aH} \frac{\partial v_x}{\partial x}, \quad (8.37)$$

with $dV_s = J dV_x$. In the second approximate equality of Eq. (8.37), we used the approximation that $aH \simeq \text{constant}$ by reflecting the fact that the region of surveys under consideration is not so large. The perturbation of the number density of galaxies in redshift space (with the average number density n_0) is given by

$$\delta_s(\mathbf{s}) = \frac{n_s dV_s}{n_0 dV_s} - 1 = \frac{n_x dV_x}{n_0 dV_s} - 1 \simeq \delta_g(\mathbf{x}) - \frac{1}{aH} \frac{\partial v_x}{\partial x}, \quad (8.38)$$

where $\delta_g(\mathbf{x}) = n_x/n_0 - 1$ is the perturbation of the number density of galaxies in real space.

On using the velocity potential v , the component v_x can be expressed by $v_x = -n^i v_{|i} = \partial v / \partial x$. We write $v(\mathbf{x})$ in terms of the sum of the Fourier modes $v(\mathbf{k})$, as

$$v(\mathbf{x}) = \frac{1}{(2\pi)^3} \int d^3k v(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}}. \quad (8.39)$$

In Fourier space, the relation (8.38) reads

$$\delta_s(\mathbf{k}) = \delta_g(\mathbf{k}) + \frac{k_x^2}{aH} v(\mathbf{k}), \quad (8.40)$$

where k_x is the x component of $\mathbf{k}$. The quantity θ defined by Eq. (8.14) reduces to $\theta(\mathbf{k}) = -k^2 v(\mathbf{k}) / (aH)$ in Fourier space, so we can express Eq. (8.40) as

$$\delta_s(\mathbf{k}, \mu) = \delta_g(\mathbf{k}) - \mu^2 \theta(\mathbf{k}), \quad (8.41)$$

where $\mu = k_x/k$ is the cosine of the angle between the momentum $\mathbf{k}$ and the x -axis. For $\mu \neq 0$, $\delta_s(\mathbf{k})$ differs from $\delta_g(\mathbf{k})$.

We define the linear galaxy power spectrum in redshift space, as $P_g^s(k, \mu) = \langle |\delta_s(\mathbf{k}, \mu)|^2 \rangle$. From Eq. (8.41), it follows that

$$P_g^s(k, \mu) = P_{gg}(k) - 2\mu^2 P_{g\theta}(k) + \mu^4 P_{\theta\theta}(k), \quad (8.42)$$

where $P_{gg}(k) \equiv \langle |\delta_g(\mathbf{k})|^2 \rangle$, $P_{g\theta}(k) \equiv \langle \delta_g(\mathbf{k}) \theta^*(\mathbf{k}) \rangle$, and $P_{\theta\theta}(k) \equiv \langle |\theta(\mathbf{k})|^2 \rangle$. $P_{gg}(k)$ is the power spectrum in real space, which corresponds to P_{δ_g} of Eq. (8.33). $P_{\theta\theta}(k)$ is the power spectrum of the peculiar velocity. $P_{g\theta}(k)$ is the cross-correlation power

spectrum between the galaxy and the peculiar velocity. On using the approximate relation (8.20), the quantity θ is related to the matter perturbation δ_m as

$$\theta \simeq -f\delta_m, \quad f \equiv \frac{\dot{\delta}_m}{H\delta_m}. \quad (8.43)$$

We apply this to Eq. (8.41) and relate δ_g to δ_m as $\delta_g = b\delta_m$ with the bias factor b . Since $\delta_s(\mathbf{k}) = b(1 + \mu^2 f/b)\delta_m(\mathbf{k})$ in Fourier space, the power spectrum (8.42) reduces to

$$P_g^s(k, \mu) = P_{gg}(k) (1 + \beta\mu^2)^2, \quad \beta \equiv \frac{f}{b}. \quad (8.44)$$

The galaxy power spectrum $P_{gg}(k)$ has the relation $P_{gg}(k) = b^2 P_{\delta_m}(k)$ with the matter power spectrum $P_{\delta_m}(k)$. The result (8.44) is known as the Kaiser formula [9]. This shows that the power spectrum in redshift space is distorted along the direction from the observer to the galaxy, which is called the redshift-space distortion (RSD).

The quantity β is related to the growth rate $\dot{\delta}_m$ of matter perturbations, so it is possible to put constraints on the cosmic growth history from RSD measurements. To see this in more detail, we expand $P_g^s(k, \mu)$ in terms of the Legendre polynomials $\mathcal{P}_l$ defined by Eq. (7.69), as

$$P_g^s(k, \mu) = \sum_{l=0}^{\infty} P_l^s(k) \mathcal{P}_l(\mu). \quad (8.45)$$

The inverse transformation gives

$$P_l^s(k) = \frac{2l+1}{2} \int_{-1}^{+1} d\mu P_g^s(k, \mu) \mathcal{P}_l(\mu). \quad (8.46)$$

The power spectrum (8.44) has only the even powers of μ . Moreover, it does not contain terms higher than the order μ^4 . This means that, for odd l and for $l > 4$, the terms $P_l^s(k)$ vanish. On using the properties $\mathcal{P}_0(\mu) = 1$, $\mathcal{P}_2(\mu) = (3\mu^2 - 1)/2$, $\mathcal{P}_4(\mu) = (35\mu^4 - 30\mu^2 + 3)/8$, the non-vanishing components of $P_l^s(k)$ are given by [10]

$$P_0^s(k) = \left(1 + \frac{2}{3}\beta + \frac{1}{5}\beta^2\right) P_{gg}(k), \quad (8.47)$$

$$P_2^s(k) = \left(\frac{4}{3}\beta + \frac{4}{7}\beta^2\right) P_{gg}(k), \quad (8.48)$$

$$P_4^s(k) = \frac{8}{35}\beta^2 P_{gg}(k). \quad (8.49)$$

From the observed power spectrum $P_g^s(k)$, it is possible to extract the information of $P_0^s(k)$ and to constrain the scale dependence of $P_{gg}(k) = b^2 P_{\delta_m}(k)$. The total amplitude of $P_{\delta_m}(k)$ depends on the amplitude of $P_{gg}(k)$ and on the bias factor b . Usually, the amplitude of $P_{\delta_m}(k)$ is normalized by the square root of the variance

$\langle |\delta_m|^2 \rangle$ of matter perturbations averaged over by the sphere with radius $8 h^{-1} \text{ Mpc}$, whose today's value is expressed as $\sigma_8(z=0)$. Assuming the flat ΛCDM model with adiabatic initial conditions of perturbations, the constraints on $\sigma_8(z=0)$ from WMAP9 and Planck 2015 data are given, respectively, by [11, 12]

$$\text{WMAP9 : } \sigma_8(z=0) = 0.821 \pm 0.023, \quad (8.50)$$

$$\text{Planck 2015 : } \sigma_8(z=0) = 0.831 \pm 0.013, \quad (8.51)$$

at 68% CL. The WMAP9 data allow smaller values of $\sigma_8(z=0)$ relative to those constrained from the Planck data.

Taking the ratio between Eqs. (8.47) and (8.48), it follows that

$$\frac{P_2^s(k)}{P_0^s(k)} = \frac{4\beta/3 + 4\beta^2/7}{1 + 2\beta/3 + \beta^2/5}, \quad (8.52)$$

which increases for larger β in the range $0 < \beta < 1$. Measuring the ratio $P_2^s(k)/P_0^s(k)$ at many different redshifts z , the quantity β associated with the growth rate of matter perturbations is constrained from the RSD data. The ratio $P_4^s(k)/P_0^s(k)$ can be also used to constrain the cosmic growth rate, but the measurements of $P_4^s(k)$ have not been accurate enough to put constraints on β .

The discussion so far is based on the linear perturbation theory. Non-linear effects come into play on small scales characterized by $k > 0.09 h^{-1} \text{ Mpc}^{-1}$. The velocity field tends to be larger due to non-linear effects, so the galaxies move outwards beyond high-density regions and hence the damping of perturbations occurs. In particular, the power spectrum of θ is damped and the relation $\theta = -f\delta_m$ starts to lose its validity. This requires the understanding of non-linear evolution of perturbations, so its modeling is generally quite complicated. One of such modeling is given by the power spectrum [13]

$$P_g^s(k, \mu) = [P_{gg}(k) - 2\mu^2 P_{g\theta}(k) + \mu^4 P_{\theta\theta}(k)] F(k, \mu), \quad (8.53)$$

where $F(k, \mu)$ characterizes the damping term. The two commonly-used forms of F are $F = [1 + (k\sigma_v\mu)^2]^{-1}$ and $F = \exp[-(k\sigma_v\mu)^2]$, where σ_v is a constant characterizing the level of damping. Empirically, it is known that the former form of F fits the data better than the latter. Taking $\sigma_v = 3 \text{ Mpc}$, $k = 0.2 h \text{ Mpc}^{-1}$, and $h = 0.7$, for example, the former damping term can be estimated as $F \simeq [1 + (0.4\mu)^2]^{-1}$.

Another modeling is given by [14, 15]

$$P_g^s(k, \mu) = b^2 P_{\delta_m}^{\text{NL}}(k) \frac{(1 + \beta\mu^2)^2}{1 + (k\sigma_v\mu)^2}, \quad (8.54)$$

where $P_{\delta_m}^{\text{NL}}$ is the power spectrum taking into account non-linear effects to the linear power spectrum P_{δ_m} . The formula was not derived theoretically, but it is useful to empirically model the nonlinear power spectrum. Computing $P_{\delta_m}^{\text{NL}}$ for a given cosmology (e.g., the ΛCDM model) and comparing $P_g^s(k, \mu)$ of Eq. (8.54) with the RSD data, it is possible to put constraints on b , f , σ_v , and $\langle |\delta_m|^2 \rangle$. From this,

we can also derive constraints on $\langle |f\delta_m|^2 \rangle$ corresponding to the power spectrum $P_{\theta\theta}$ in the linear perturbation theory. Besides Eq. (8.54), there were also attempts for theoretically constructing $P_g^s(k, \mu)$ by extending the linear perturbation theory to a quasi-nonlinear regime [16, 17] and for placing constraints on the growth rate by using the fitting formulas of $P_{\theta\theta}$ etc extracted from N -body simulations [18].

8.5. Constraints on the cosmic growth rate from RSD measurements

In Sec. 8.4, we have studied how the matter perturbation δ_m and its growth rate $\dot{\delta}_m$ can be constrained from the observations of RSD. The RSD data can be used to place constraints on the property of dark energy. In doing so, we will derive analytic solutions to δ_m and $f = \dot{\delta}_m/(H\delta_m)$ for dark energy models with constant w_{DE} .

In the presence of non-relativistic matter and dark energy, we have $\dot{H} = -4\pi G[\rho_m + (1 + w_{\text{DE}})\rho_{\text{DE}}]$ and $\dot{\rho}_{\text{DE}} + 3H(1 + w_{\text{DE}})\rho_{\text{DE}} = 0$ from Eqs. (4.19) and (4.20), respectively. Using the dark energy density parameter Ω_{DE} , they can be expressed as

$$\frac{\dot{H}}{H^2} = -\frac{3}{2}(1 + w_{\text{DE}}\Omega_{\text{DE}}), \quad (8.55)$$

$$\dot{\Omega}_{\text{DE}} = -3Hw_{\text{DE}}\Omega_{\text{DE}}(1 - \Omega_{\text{DE}}), \quad (8.56)$$

where we used $\Omega_m = 1 - \Omega_{\text{DE}}$. Ignoring the contribution of dark energy perturbations in Eq. (8.30) and expressing this equation with respect to $f = \dot{\delta}_m/(H\delta_m)$, it follows that

$$\frac{\dot{f}}{H} + \left(2 + f + \frac{\dot{H}}{H^2}\right)f - \frac{3}{2}(1 - \Omega_{\text{DE}}) = 0. \quad (8.57)$$

The matter perturbation equation does not have scale dependence in linear perturbation theory. On using Eqs. (8.55) and (8.56) in Eq. (8.57), we obtain

$$3w_{\text{DE}}\Omega_{\text{DE}}(1 - \Omega_{\text{DE}})\frac{df}{d\Omega_{\text{DE}}} = f^2 + \frac{1}{2}(1 - 3w_{\text{DE}}\Omega_{\text{DE}})f - \frac{3}{2}(1 - \Omega_{\text{DE}}). \quad (8.58)$$

We define the growth index γ in the form of

$$f = (\Omega_m)^\gamma = (1 - \Omega_{\text{DE}})^\gamma. \quad (8.59)$$

Then, Eq. (8.58) reduces to

$$\begin{aligned} & 3w_{\text{DE}}\Omega_{\text{DE}}(1 - \Omega_{\text{DE}})\ln(1 - \Omega_{\text{DE}})\frac{d\gamma}{d\Omega_{\text{DE}}} \\ &= \frac{1}{2} - \frac{3}{2}w_{\text{DE}}(1 - 2\gamma)\Omega_{\text{DE}} + (1 - \Omega_{\text{DE}})^\gamma - \frac{3}{2}(1 - \Omega_{\text{DE}})^{1-\gamma}. \end{aligned} \quad (8.60)$$

Dealing with Ω_{DE} as a small expansion parameter, we expand the growth index as

$$\gamma = \gamma_0 + \sum_{n=1}^{\infty} \gamma_n (\Omega_{\text{DE}})^n. \quad (8.61)$$

Substituting Eq. (8.61) into Eq. (8.60), we can derive the coefficients $\gamma_0, \gamma_1, \dots$ iteratively. Up to the second-order expansion in Ω_{DE} , the growth index can be expressed as [19]

$$\begin{aligned} \gamma = & \frac{3(1-w_{\text{DE}})}{5-6w_{\text{DE}}} + \frac{3}{2} \frac{(1-w_{\text{DE}})(2-3w_{\text{DE}})}{(5-6w_{\text{DE}})^2(5-12w_{\text{DE}})} \Omega_{\text{DE}} \\ & + \frac{(w_{\text{DE}}-1)(3w_{\text{DE}}-2)(324w_{\text{DE}}^2-420w_{\text{DE}}+97)}{4(5-6w_{\text{DE}})^3(5-12w_{\text{DE}})(5-18w_{\text{DE}})} \Omega_{\text{DE}}^2 + \mathcal{O}(\Omega_{\text{DE}}^3). \end{aligned} \quad (8.62)$$

For $w_{\text{DE}} = -1$, we have $\gamma \simeq 0.545 + 7.29 \times 10^{-3} \Omega_{\text{DE}} + 4.04 \times 10^{-3} \Omega_{\text{DE}}^2$, which is nearly constant: $\gamma \simeq 0.545$. If w_{DE} is larger than -1 , the growth index tends to be larger, e.g., $\gamma = 0.554$ for $w_{\text{DE}} = -0.7$. Then, γ is not very much different from the value for $w_{\text{DE}} = -1$. Provided that w_{DE} slowly varies in time around -1 , the growth index is nearly constant with $\gamma \simeq 0.55$ [20]. In modified gravitational theories, however, γ generally deviates from 0.55 [21, 22].

On using Eq. (8.56), the relation $f = (1 - \Omega_{\text{DE}})^\gamma$ can be expressed as

$$\frac{d}{d\Omega_{\text{DE}}} \ln \delta_m = -\frac{(1 - \Omega_{\text{DE}})^{\gamma-1}}{3w_{\text{DE}}\Omega_{\text{DE}}}. \quad (8.63)$$

We expand the term $(1 - \Omega_{\text{DE}})^{\gamma-1}$ in the form

$$(1 - \Omega_{\text{DE}})^{\gamma-1} = 1 + \sum_{n=1}^{\infty} c_n (\Omega_{\text{DE}})^n, \quad c_n = \frac{(-1)^n}{n!} \prod_{i=1}^n (\gamma - i). \quad (8.64)$$

Assuming that γ is constant, we can integrate Eq. (8.63) to give

$$\delta_m = \delta_m^{(0)} \exp \left\{ \frac{1}{3w_{\text{DE}}} \left[\ln \frac{\Omega_{\text{DE}}^{(0)}}{\Omega_{\text{DE}}} + \sum_{n=1}^{\infty} \frac{c_n}{n} \left((\Omega_{\text{DE}}^{(0)})^n - (\Omega_{\text{DE}})^n \right) \right] \right\}, \quad (8.65)$$

where $\delta_m^{(0)}$ is the present value of δ_m . Normalizing $\delta_m^{(0)}$ by $\sigma_8(z=0)$, the value of $f\sigma_8$ at the redshift z can be expressed as [23]

$$\begin{aligned} f\sigma_8(z) = & (1 - \Omega_{\text{DE}})^\gamma \sigma_8(z=0) \\ & \times \exp \left\{ \frac{1}{3w_{\text{DE}}} \left[\ln \frac{\Omega_{\text{DE}}^{(0)}}{\Omega_{\text{DE}}} + \sum_{n=1}^{\infty} \frac{c_n}{n} \left((\Omega_{\text{DE}}^{(0)})^n - (\Omega_{\text{DE}})^n \right) \right] \right\}. \end{aligned} \quad (8.66)$$

The quantity $f\sigma_8(z)$, which is related to the power spectrum $P_{\theta\theta}$ of peculiar velocities discussed in Sec. 8.4, corresponds to the product of $\beta = f/b$ and the square root $b\sigma_8$ of the galaxy power spectrum P_{gg} at the scale $8h^{-1} \text{Mpc}$. This

quantity is not affected by the uncertainty of the bias factor b . Since the densities of dark energy and non-relativistic matter at the redshift z are given, respectively, by $\rho_{\text{DE}} = \rho_{\text{DE}}^{(0)}(1+z)^{3(1+w_{\text{DE}})}$ and $\rho_m = \rho_m^{(0)}(1+z)^3$, the density parameter Ω_{DE} in Eq. (8.66) can be expressed as

$$\Omega_{\text{DE}}(z) = \frac{\Omega_{\text{DE}}^{(0)}(1+z)^{3w_{\text{DE}}}}{1 - \Omega_{\text{DE}}^{(0)} + \Omega_{\text{DE}}^{(0)}(1+z)^{3w_{\text{DE}}}}. \quad (8.67)$$

The constant c_n in Eq. (8.64) contains the growth index γ , which depends on w_{DE} and Ω_{DE} as Eq. (8.62). On using Eq. (8.67), the quantity $f\sigma_8(z)$ of Eq. (8.66) is expressed in terms of the three parameters w_{DE} , $\Omega_{\text{DE}}^{(0)}$, and $\sigma_8(z=0)$. Since the evolution of $f\sigma_8(z)$ is different depending on the values of w_{DE} , it is possible to place observational constraints on w_{DE} from RSD measurements.

In Fig. 8.5, we plot the evolution of $f(z)\sigma_8(z)$ derived by the analytic solution (8.66) for several different values of w_{DE} with $\sigma_8(z=0) = 0.811$. The thin solid lines show the numerically integrated solutions to Eq. (8.57) with the initial condition $f = 1$. The analytic solutions (bold dashed lines in Fig. 8.5) up to $n = 7$ terms of Eq. (8.66) exhibit good agreement with the numerical results. For smaller w_{DE} the cosmic acceleration is stronger, so the decrease of $f\sigma_8$ for $z \lesssim 0.5$ tends to be more significant.

In Fig. 8.6, we show $f(z)\sigma_8(z)$ versus z for the best-fit Λ CDM model ($w_{\text{DE}} = -1$) with $\sigma_8(z=0)$ constrained from the WMAP9 and Planck 2015 data. On using

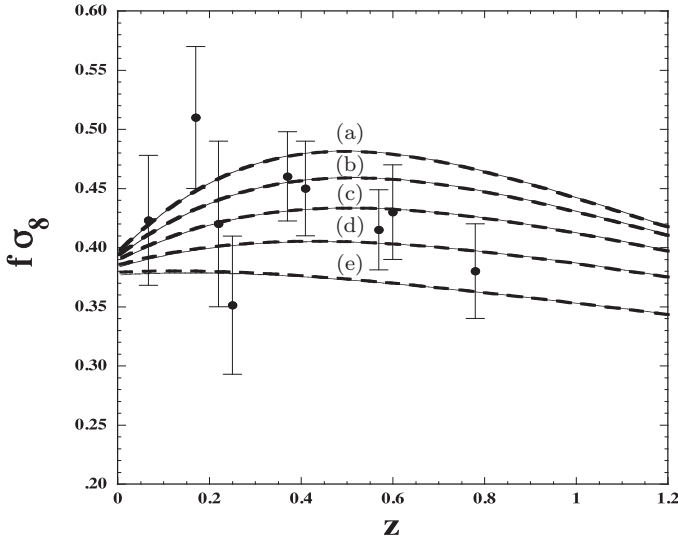


Fig. 8.5. Evolution of $f\sigma_8$ versus z for the models with $c_s^2 = 1$ and (a) $w = -1.2$, (b) $w = -1$, (c) $w = -0.8$, (d) $w = -0.6$, (e) $w = -0.4$, respectively, with $\sigma_8(z=0) = 0.811$. The solid lines correspond to the numerically integrated solutions, whereas the bold dashed lines are derived from the analytic estimation (8.66) with the 7-th order terms of c_n . The RSD data are also shown with error bars. Reproduced from Ref. [23].

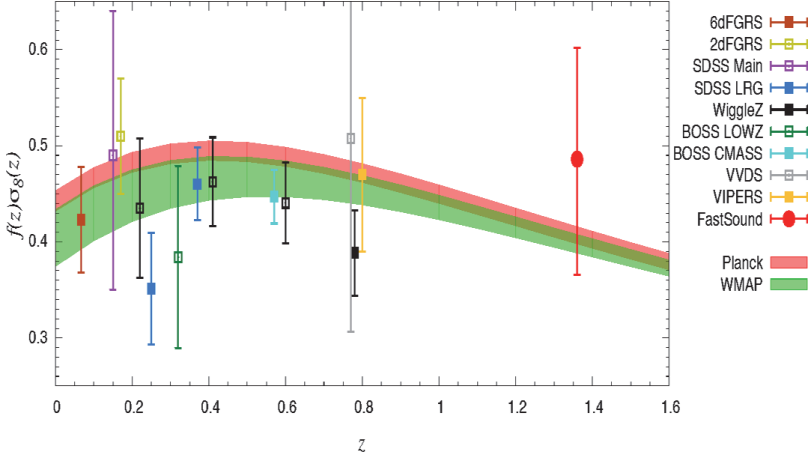


Fig. 8.6. Constraints on the growth rate $f(z)\sigma_8(z)$ as a function of z in the best-fit Λ CDM model. We show theoretical predictions with 68% confidence intervals based on WMAP9 and Planck CMB measurements of $\sigma_8(z=0)$. The RSD data, which include the FastSound data at $z=1.4$ [24], are plotted with error bars. The author thanks Teppei Okumura for providing this figure.

the WMAP9 bound (8.50) of $\sigma_8(z=0)$, the RSD data of $f(z)\sigma_8(z)$ plotted in Fig. 8.6 are consistent with the theoretical prediction of the Λ CDM model. This can be also confirmed in Fig. 8.5 in which the chosen value $\sigma_8(z=0) = 0.811$ is within the WMAP9 bound.

From Eq. (8.51), the Planck 2015 data favor larger values of $\sigma_8(z=0)$ than those constrained from the WMAP9 data. Moreover, the density parameter of non-relativistic matter constrained from the Planck 2015 data is around $\Omega_m^{(0)} \simeq 0.32$, which is larger than the WMAP9 best-fit value $\Omega_m^{(0)} \simeq 0.28$. As we see in Fig. 8.6, the values of $f(z)\sigma_8(z)$ predicted by using the Planck 2015 bound of $\sigma_8(z=0)$ are larger than those derived by employing the WMAP9 bound of $\sigma_8(z=0)$. With the Planck 2015 data of $\sigma_8(z=0)$, the theoretical values of $f(z)\sigma_8(z)$ in the Λ CDM model is in mild tension with the RSD data in the low-redshift regime. The measurement of $f(z)\sigma_8(z)$ at $z=1.4$ by FastSound [24] is consistent with the prediction of the Λ CDM model. So far, the RSD measurements have not been accurate enough to place tight constraints on the property of dark energy. However, this situation will be improved in future high-precision observations like the Euclid mission.¹

8.6. BAO

Before the CMB decoupling epoch the baryon was tightly coupled to the photon, so from Eq. (7.117) the baryon perturbation δ_b was related to the monopole component Θ_0 of temperature perturbations as $\delta_b = 3\Theta_0$. In this epoch the

¹See <http://sci.esa.int/euclid/>.

baryon perturbation exhibited acoustic oscillations, but it started to grow after the decoupling with photons. Analogous to the acoustic oscillations of photons measured in the observations of CMB temperature anisotropies, there should be imprints of the oscillations of baryon perturbations in the observation of large-scale structures. The baryon acoustic oscillation was first measured in 2005 from the observations of two-point correlation functions in the spatial distribution of galaxies [25].

For the perturbation $\delta(\mathbf{x})$ at a given point $\mathbf{x}$ the two-point correlation function is defined by $\xi(s) = \langle \delta(\mathbf{x}_1) \delta(\mathbf{x}_2) \rangle$, where $s = |\mathbf{x}_1 - \mathbf{x}_2|$. The power spectrum $P(k)$ corresponds to the Fourier transform of $\xi(s)$, so that

$$\xi(s) = \frac{1}{(2\pi)^3} \int d^3k P(k) e^{i\mathbf{k} \cdot \mathbf{s}}. \quad (8.68)$$

In Fig. 8.7, we plot the two-point correlation function $\xi(s)$ of the galaxy distribution in redshift space derived from SDSS surveys [25]. The power spectrum associated with $\xi(s)$ corresponds to $P_0^s(k)$ given by Eq. (8.47). The observational data in Fig. 8.7 show a peak around the coming scale $s = 100 h^{-1} \text{ Mpc}$ induced by baryon acoustic oscillations.

As in the case of temperature anisotropies, the quantity characterizing the peak position is the sound horizon $r_s(\eta_*)$ at the CMB decoupling epoch. The peak of oscillations arises at the position satisfying Eq. (7.175). Strictly speaking, the redshift z_b at which baryons were decoupled from photons is different from the redshift z_* at which free electrons were decoupled from photons. As in the case of z_* in Eq. (7.15),

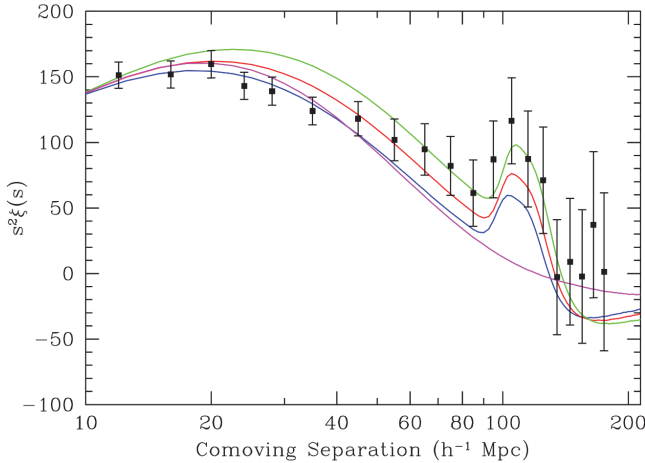


Fig. 8.7. The large-scale correlation function $\xi(s)$ of the SDSS LRG galaxy sample multiplied by the distance squared s^2 . The three solid curves with peaks correspond to $\Omega_m^{(0)} h^2 = 0.12, 0.13, 0.14$ from top to bottom with $\Omega_b^{(0)} h^2 = 0.024$, while the solid curve at the bottom corresponds to $\Omega_m^{(0)} h^2 = 0.105$ and $\Omega_b^{(0)} h^2 = 0$. The observational data of $s^2 \xi(s)$ show a peak of baryon acoustic oscillations around the scale $100 h^{-1} \text{ Mpc}$. Reproduced from Ref. [25].

there is the fitting formula of z_b as [26]

$$z_b = \frac{1291\omega_m^{0.251}}{1 + 0.659\omega_m^{0.828}}(1 + b_1\omega_b^{b_2}), \quad (8.69)$$

where

$$b_1 = 0.313\omega_m^{-0.419}(1 + 0.607\omega_m^{0.674}), \quad b_2 = 0.238\omega_m^{0.223}. \quad (8.70)$$

Using the central values of the present density parameters of baryons and CDM given by Eqs. (4.63) and (4.67), we have $\omega_b = \Omega_b^{(0)}h^2 = 0.02205$ and $\omega_m = \Omega_c^{(0)}h^2 + \Omega_b^{(0)}h^2 = 0.14195$, in which case $z_b \simeq 1020$. This is smaller than the value $z_* \simeq 1090$ derived from Eq. (7.15).

Analogous to Eq. (7.178), the sound horizon at $z = z_b$ reads

$$r_s(z_b) = \frac{4}{3} \frac{h}{H_0} \sqrt{\frac{\omega_\gamma}{\omega_m \omega_b}} \ln \left(\frac{\sqrt{R_s(z_b) + R_s(z_{\text{eq}})} + \sqrt{1 + R_s(z_b)}}{1 + \sqrt{R_s(z_{\text{eq}})}} \right), \quad (8.71)$$

where z_{eq} is given by Eq. (4.80). The quantity R_s , which is defined by Eq. (7.163), can be expressed as $(3\omega_b/4\omega_\gamma)/(1+z)$. Since $\omega_\gamma = 2.47 \times 10^{-5}$ from Eq. (4.28), we have $R_s(z_{\text{eq}}) = 0.197$ and $R_s(z_b) = 0.656$ for $\omega_b = 0.02205$. Using Eq. (2.10) and substituting the value $h = 0.68$ into Eq. (8.71), we obtain $r_s(z_b) \simeq 103 h^{-1} \text{Mpc}$ from Eq. (8.71). This matches with the peak position of large-scale correlation functions shown in Fig. 8.7.

The wavenumber associated with the BAO acoustic peak corresponds to $k \approx 0.01 h \text{Mpc}^{-1}$. This is considerably a large scale at which the linear perturbation theory does not lose its validity for the matter power spectrum shown in Fig. 8.4. As in the case of photon perturbations, the baryon perturbation is subject to the Silk damping on small scales, whose typical damping scale is less than 10 Mpc. On such small scales, the CDM perturbation is the main contribution to the galaxy power spectrum.

From Eq. (8.36), the redshift $\delta z_s(z)$ corresponding to the sound horizon $r_s(z_b)$ along the line-of-sight direction from the observer to the galaxy in redshift space is given by

$$\delta z_s(z) = r_s(z_b) H(z). \quad (8.72)$$

The visual angle $\theta_s(z)$ of the length scale $r_s(z_b)$ orthogonal to the line-of-sight direction reads

$$\theta_s(z) = \frac{r_s(z_b)}{(1+z)d_A(z)}, \quad (8.73)$$

where $d_A(z)$ is the angular diameter distance defined by Eq. (4.9) and $(1+z)d_A(z)$ is the coming angular diameter distance $D_A(z)$. For the flat Universe ($\mathcal{K} = 0$), we have $(1+z)d_A(z) = \int_0^z d\tilde{z}/H(\tilde{z})$ from Eq. (4.8). The present BAO observations are not accurate enough to extract constraints on $H(z)$ and $d_A(z)$ independently from

Table 8.1. BAO data derived in several LSS surveys.

Redshift	$r_s(z_b)/D_V(z)$	Surveys
0.1	0.336 ± 0.015	6dFGS
0.35	0.113 ± 0.002	SDSS-DR7
0.57	0.073 ± 0.001	SDSS-DR9
0.44	0.0916 ± 0.0071	WiggleZ
0.60	0.0726 ± 0.0034	WiggleZ
0.73	0.0592 ± 0.0032	WiggleZ

Eqs. (8.72) and (8.73), respectively [27]. Instead, the power spectrum averaged over in the three-dimensional space defined by

$$[\theta_s^2(z)\Delta_s(z)]^{1/3} = \frac{r_s(z_b)}{[(1+z)^2 d_A^2(z) H^{-1}(z)]^{1/3}} \quad (8.74)$$

is used for the estimation of the distance to galaxies.

In actual observations, the following quantity is often used for BAO distance measurements:

$$D_V(z) \equiv [(1+z)^2 d_A^2(z) z H^{-1}(z)]^{1/3}, \quad (8.75)$$

which is associated with the denominator of Eq. (8.74). The constraints on the ratio $r_s(z_b)/D_V(z)$ can be derived from the BAO observations. In Table 8.1, we show the BAO data sets used in the WMAP9 analysis derived from 6dFGS [28], SDSS-DR7 [29], SDSS-DR9 [30], and WiggleZ surveys [31].² These data can be incorporated into a likelihood analysis of the form [11]

$$\chi_{\text{BAO}}^2 = (\mathbf{x} - \mathbf{d})^T \mathbf{C}^{-1} (\mathbf{x} - \mathbf{d}), \quad (8.76)$$

where the vector $\mathbf{x} - \mathbf{d}$ is given by

$$\begin{aligned} \mathbf{x} - \mathbf{d} = & [r_s(z_b)/D_V(0.1) - 0.336, D_V(0.35)/r_s(z_b) - 8.88, \\ & D_V(0.57)/r_s(z_b) - 13.67, r_s(z_b)/D_V(0.44) - 0.0916, \\ & r_s(z_b)/D_V(0.60) - 0.0726, r_s(z_b)/D_V(0.73) - 0.0592], \end{aligned} \quad (8.77)$$

and the inverse of the covariance matrix

$$\mathbf{C}^{-1} = \begin{pmatrix} 4444.4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 34.602 & 0 & 0 & 0 & 0 \\ 0 & 0 & 20.661157 & 0 & 0 & 0 \\ 0 & 0 & 0 & 24532.1 & -25137.7 & 12099.1 \\ 0 & 0 & 0 & -25137.7 & 134598.4 & -64783.9 \\ 0 & 0 & 0 & 12099.1 & -64783.9 & 128837.6 \end{pmatrix}. \quad (8.78)$$

²The SDSS-DR7 and SDSS-DR9 data have been inverted from the published values: $D_V(0.35)/r_s(z_b) = 8.88 \pm 0.17$ [29] and $D_V(0.57)/r_s(z_b) = 13.67 \pm 0.22$ [30].

The joint likelihood analysis of SN Ia, CMB, and BAO can be carried out by computing the total χ^2 defined by

$$\chi^2 = \chi_{\text{SN Ia}}^2 + \chi_{\text{CMB}}^2 + \chi_{\text{BAO}}^2. \quad (8.79)$$

The best-fit model parameters can be found by minimizing χ^2 .

In Fig. 8.2, we show observational bounds on w_{DE} and $\Omega_m^{(0)}$ derived by the data analysis of BAO combined with SN Ia and CMB (from WMAP) data for the constant w_{DE} model. The Λ CDM model ($w_{\text{DE}} = -1$) is consistent with the BAO measurements for $0.24 < \Omega_m^{(0)} < 0.33$ (95% CL). The joint data analysis of SN Ia+WMAP+BAO show that the dark energy equation of state is constrained to be $-1.2 < w_{\text{DE}} < -0.8$ (95% CL). This is also consistent with Planck+WP+BAO and Planck+WP+JLA contours plotted in Fig. 5.3. For the CPL parameterization (5.23), we observe in Fig. 5.4 that adding the BAO data to the Planck+WP+JLA data gives tighter bounds on w_0 and w_a . These parameters are constrained to be $-1.1 < w_0 < -0.75$ and $-1.3 < w_a < 0.25$ (68% CL) from the combined data analysis of Planck+WP+BAO+JLA. Thus, the Λ CDM model is consistent with the joint constraints from CMB+BAO+SN Ia, but the current data also allow the deviation of w_{DE} from -1 .

8.7. Weak lensing

Another observational probe of dark energy is a phenomenon called weak lensing [32]. If there are objects with strong gravitational fields between a source and an observer, the path of light is bent by the gravitational field. Then, the image of source seen by the observer is subject to change. While the shape of source changes significantly in strong lensing, the distortion of source is small in weak lensing. The probability that strong lensing is observed is low because this requires that the source and the lensing object (which is the gravitational source responsible for the distortion) exist practically along the same parallel direction. In weak lensing the distortion of each source is small, but it is possible to extract information of the mass distribution statistically by surveying how galaxies are distorted statistically. This information can be used for estimating the matter power spectrum. In what follows, we explain the basics of weak lensing.

As we showed in Eq. (3.66), the photon obeys the geodesic equation

$$\frac{dP^\mu}{d\lambda} + \Gamma_{\alpha\beta}^\mu \frac{dx^\alpha}{d\lambda} \frac{dx^\beta}{d\lambda} = 0, \quad (8.80)$$

where P^μ is the four-momentum defined by Eq. (7.19) and λ is the Affine parameter. From Eq. (7.20) we have the relation $g_{\mu\nu}P^\mu P^\nu = 0$ for photons. We choose the perturbed metric (7.17) in the Newtonian gauge, i.e.,

$$ds^2 = a^2(\eta) [-(1 + 2\Psi)d\eta^2 + (1 + 2\Phi)\delta_{ij}dx^i dx^j]. \quad (8.81)$$

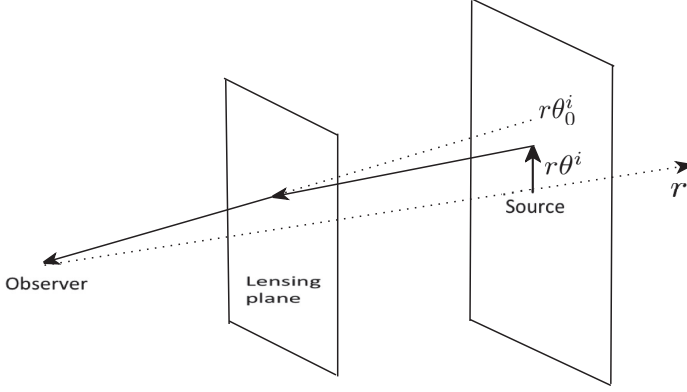


Fig. 8.8. Sketch of weak gravitational lensing. The light emitted from the point r^i is bent by the lensing object. From the observer, it looks like an image located at the point r_0^i .

We study how the source is distorted by the weak gravitational lensing associated with two gravitational potentials Ψ and Φ . On the background without perturbations, we have $\Gamma_{00}^0 = \mathcal{H}$ and $\Gamma_{ij}^0 = \mathcal{H}\delta_{ij}$, so Eq. (8.80) yields

$$\frac{dP^0}{d\lambda} + \mathcal{H}[(P^0)^2 + \delta_{ij}P^iP^j] = 0. \quad (8.82)$$

Using the relations $\delta_{ij}P^iP^j = (P^0)^2$ and $d/d\lambda = P^0(d/d\eta)$, Eq. (8.82) reduces to

$$\frac{dP^0}{d\eta} = -2\mathcal{H}P^0. \quad (8.83)$$

The solution to this equation is given by $P^0 = Ca^{-2}$, where C is an integration constant.

We take the radial direction ($r = x^3$) from an observer to a source and consider a two-dimensional plane with the coordinate (x_1, x_2) orthogonal to the r direction (see Fig. 8.8). Writing the geodesic equations (8.80) for x_i (with $i = 1, 2$) up to first order in x^i , it follows that

$$\frac{d^2x^i}{d\lambda^2} + \Gamma_{00}^i \left(\frac{d\eta}{d\lambda} \right)^2 + 2\Gamma_{0j}^i \frac{d\eta}{d\lambda} \frac{dx^j}{d\lambda} + \Gamma_{33}^i \left(\frac{dr}{d\lambda} \right)^2 = 0. \quad (8.84)$$

The Christoffel symbols are given by $\Gamma_{00}^i = \Psi_{,i}$, $\Gamma_{0j}^i = \mathcal{H}\delta_j^i$, and $\Gamma_{33}^i = -\Phi_{,i}$, where we dropped the perturbed part of Γ_{0j}^i . Setting $ds^2 = 0$ in Eq. (8.81), we obtain $dr = (1 - \Phi + \Psi)d\eta$ at linear order in perturbations. Hence Eq. (8.84) reduces to

$$\frac{d^2x^i}{d\lambda^2} + 2\mathcal{H} \frac{d\eta}{d\lambda} \frac{dx^i}{d\lambda} = \left(\frac{d\eta}{d\lambda} \right)^2 (\Phi_{,i} - \Psi_{,i}), \quad (8.85)$$

where the right hand side corresponds to the first-order quantity. Employing Eq. (8.83) and the approximation $dr \simeq d\eta$, it follows that $dx^i/d\lambda \simeq P^0(dx^i/dr)$

and

$$\frac{d^2 x^i}{d\lambda^2} = (P^0)^2 \frac{d^2 x^i}{dr^2} - 2\mathcal{H}P^0 \frac{dx^i}{d\lambda}. \quad (8.86)$$

Then, Eq. (8.85) yields

$$\frac{d^2 x^i}{dr^2} = \psi_{\text{eff},i}, \quad \psi_{\text{eff}} \equiv \Phi - \Psi, \quad (8.87)$$

where ψ_{eff} is the effective gravitational potential characterizing the deviation of light rays in weak lensing observations. In the absence of the anisotropic stress we have $\Psi = -\Phi$, in which case $\psi_{\text{eff}} = 2\Phi$. If Φ increases toward the central direction at the origin ($x^1 = x^2 = 0$), it follows that $\psi_{\text{eff},i} < 0$. In this case, the light is bent inward from Eq. (8.87).

The amplitude of the vector $\mathbf{x} = (x^1, x^2)$ is small in weak lensing measurements, so we can set $x^i = r\theta^i$ in Eq. (8.87). Integrating Eq. (8.87) twice with respect to r , it follows that

$$\theta^i = \theta_0^i + \frac{1}{r} \int_0^r dr'' \int_0^{r''} dr' \psi_{\text{eff},i}(r'), \quad (8.88)$$

where θ_0^i is the value of θ^i for $\psi_{\text{eff}} = 0$, i.e., the angle of image measured by the observer. The regions of integral (8.88) with respect to r'' and r' correspond to $0 < r'' < r$ and $0 < r' < r''$, respectively, so this is equivalent to integrals in the regions $r' < r'' < r$ and $0 < r' < r$. Performing the integral with respect to r'' , we obtain

$$\theta^i = \theta_0^i + \int_0^r dr' \left(1 - \frac{r'}{r}\right) \psi_{\text{eff},i}(r'). \quad (8.89)$$

The mapping from the angular coordinate θ_0^j (with $j = 1, 2$) of the observed image to the angular coordinate θ^i (with $i = 1, 2$) is given by

$$A_{ij} = \frac{\partial \theta^i}{\partial \theta_0^j} = \delta_{ij} + \int_0^r dr' r' \left(1 - \frac{r'}{r}\right) \psi_{\text{eff},ij}(r'), \quad (8.90)$$

where A_{ij} 's are components of the 2×2 symmetric matrix A with three independent components κ , γ_1 , γ_2 . The matrix A can be expressed in the form

$$A = \begin{pmatrix} 1 - \kappa - \gamma_1 & -\gamma_2 \\ -\gamma_2 & 1 - \kappa + \gamma_1 \end{pmatrix}, \quad (8.91)$$

where

$$\kappa = -\frac{1}{2} \int_0^r dr' r' \left(1 - \frac{r'}{r}\right) (\psi_{\text{eff},11} + \psi_{\text{eff},22}), \quad (8.92)$$

$$\gamma_1 = -\frac{1}{2} \int_0^r dr' r' \left(1 - \frac{r'}{r}\right) (\psi_{\text{eff},11} - \psi_{\text{eff},22}), \quad (8.93)$$

$$\gamma_2 = - \int_0^r dr' r' \left(1 - \frac{r'}{r}\right) \psi_{\text{eff},12}. \quad (8.94)$$

The quantity κ , which is called a convergence field, plays the role of changing the area while keeping the isotropy of the image. On the other hand, if γ_1 increases (decreases), then A_{11} decreases (increases) while A_{22} increases (decreases). This means that the term γ_1 gives rise to an anisotropic distortion in the $\boldsymbol{\theta} = (\theta^1, \theta^2)$ coordinate plane. Similarly, the term γ_2 leads to a distortion in the direction inclined by the angle $\pi/4$ from the θ^1 axis. The quantities γ_1 and γ_2 are called shear fields.

Equations (8.92)–(8.94) contain the spatial derivative of $\psi_{\text{eff}} = \Phi - \Psi$. We introduce the effective density field δ_{eff} related to ψ_{eff} as

$$\nabla^2 \psi_{\text{eff}} = -3H_0^2 \Omega_m^{(0)} \frac{\delta_{\text{eff}}}{a}, \quad (8.95)$$

where $\Omega_m^{(0)}$ is the density parameter of non-relativistic matter, and the scale factor a is normalized as $a_0 = 1$ today. In GR the gravitational potential Φ is related to the matter perturbation δ_m through the Poisson equation (6.130) with $\mathcal{K} = 0$. Moreover, there is the relation $\Psi = -\Phi$ after the end of the radiation era by neglecting the neutrino's anisotropic stress. We also have $\Omega_m^{(0)} = 8\pi G \rho_0 / (3H_0^2)$ with $\rho = \rho_0 a^{-3}$, so δ_{eff} is equivalent to the gauge-invariant density contrast δ_m . In modified gravity theories, δ_{eff} is not generally identical to δ_m .

In terms of δ_{eff} , Eq. (8.92) can be expressed as

$$\kappa(\boldsymbol{\theta}) = \frac{3H_0^2 \Omega_m^{(0)}}{2} \int_0^r dr' \frac{r'(r-r')}{r} \frac{\delta_{\text{eff}}(\mathbf{r}')}{a(r')}. \quad (8.96)$$

For a distributed lensing source, we consider the distribution function $n(r)$ normalized by the condition $\int_0^\infty dr n(r) = 1$. In this case, we only need to change Eq. (8.96) to $\int_0^\infty dr n(r) \kappa(\boldsymbol{\theta})$. Then, the convergence field reduces to

$$\begin{aligned} \kappa(\boldsymbol{\theta}) &= \frac{3H_0^2 \Omega_m^{(0)}}{2} \int_0^\infty dr n(r) \int_0^r dr' \frac{r'(r-r')}{r} \frac{\delta_{\text{eff}}(\mathbf{r}')}{a(r')} \\ &= \frac{3H_0^2 \Omega_m^{(0)}}{2} \int_0^\infty dr r \frac{\delta_{\text{eff}}(\mathbf{r}) g(r)}{a(r)}, \end{aligned} \quad (8.97)$$

where

$$g(r) = \int_r^\infty dr' \frac{r' - r}{r'} n(r'). \quad (8.98)$$

In deriving Eq. (8.97), we changed the r integral in the region $0 < r < \infty$ and the r' integral in the region $0 < r' < r$ to those in the regions $r' < r < \infty$ and $0 < r' < \infty$,

respectively, and finally exchanged r and r' . If the source is located around $r' = r_s$ in Eq. (8.98), it follows that $n(r') = \delta(r' - r_s)$ and hence $g(r) = (r_s - r)/r_s$.

We perform the Fourier transformation of $\kappa(\boldsymbol{\theta})$ in Eq. (8.97) in the two-dimensional $\boldsymbol{\theta} = (\theta^1, \theta^2)$ plane and write the Fourier components as

$$\kappa_l = \int d^2\boldsymbol{\theta} \kappa(\boldsymbol{\theta}) e^{-i\mathbf{l}\cdot\boldsymbol{\theta}}, \quad (8.99)$$

where $\mathbf{l}$ is the two-dimensional vector of wavenumber. Then, the power spectrum $P_\kappa(l)$ of the two-dimensional convergence field is defined by

$$\langle \kappa_l \kappa_{l'}^* \rangle = (2\pi)^2 \delta^{(2)}(\mathbf{l} - \mathbf{l}') P_\kappa(l), \quad (8.100)$$

where $\delta^{(2)}(\mathbf{l} - \mathbf{l}')$ is a two-dimensional delta function. The effective density field $\delta_{\text{eff}}(\mathbf{r})$ appearing in Eq. (8.97) depends on both r and $r\boldsymbol{\theta}$. Expressing the corresponding wavenumbers of r and $r\boldsymbol{\theta}$ as k_r and $\mathbf{k}_\theta$, respectively, we can write $\delta_{\text{eff}}(\mathbf{r})$ in Fourier series, as

$$\delta_{\text{eff}}(\mathbf{r}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \delta_{\mathbf{k}} e^{ik_r r} e^{i\mathbf{k}_\theta \cdot r\boldsymbol{\theta}}. \quad (8.101)$$

Then, Eq. (8.99) reduces to

$$\kappa_l = \frac{3H_0^2 \Omega_m^{(0)}}{2} \int_0^\infty dr \mathcal{G}(r) \int d^2\boldsymbol{\theta} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \delta_{\mathbf{k}} e^{ik_r r} e^{i\mathbf{k}_\theta \cdot r\boldsymbol{\theta}} e^{-i\mathbf{l}\cdot\boldsymbol{\theta}}, \quad (8.102)$$

where $\mathcal{G}(r) \equiv rg(r)/a(r)$. On using the fact that $k_r \ll k_\theta \equiv |\mathbf{k}_\theta|$ in realistic surveys and that $\delta(r - r') = \frac{1}{2\pi} \int dk_r e^{ik_r(r-r')}$, we obtain

$$\begin{aligned} \langle \kappa_l \kappa_{l'}^* \rangle &= \frac{1}{(2\pi)^2} \left(\frac{3H_0^2 \Omega_m^{(0)}}{2} \right)^2 \int_0^\infty dr \mathcal{G}(r) \int_0^\infty dr' \mathcal{G}(r') \delta(r' - r) \\ &\quad \times \int d^2\mathbf{k}_\theta P_{\delta_{\text{eff}}}(k_\theta, r) \int d^2\boldsymbol{\theta} e^{i(\mathbf{k}_\theta r - \mathbf{l}) \cdot \boldsymbol{\theta}} \int d^2\boldsymbol{\theta}' e^{-i(\mathbf{k}_\theta r' - \mathbf{l}') \cdot \boldsymbol{\theta}'}, \end{aligned} \quad (8.103)$$

where $P_{\delta_{\text{eff}}}$ is the power spectrum of the effective density field defined by

$$\langle \delta_{\mathbf{k}} \delta_{\mathbf{k}'}^* \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{k} - \mathbf{k}') P_{\delta_{\text{eff}}}(k). \quad (8.104)$$

In Eq. (8.103), we have explicitly written the r dependence in P_{δ_m} . On using the property $\int d^2\boldsymbol{\theta} e^{i(\mathbf{k}_\theta r - \mathbf{l}) \cdot \boldsymbol{\theta}} = (2\pi)^2 \delta^{(2)}(\mathbf{k}_\theta r - \mathbf{l}) = (2\pi)^2 \delta^{(2)}(\mathbf{k}_\theta - \mathbf{l}/r)/r$, non-vanishing contributions to the $\mathbf{k}_\theta$ integral in Eq. (8.103) correspond to $\mathbf{k}_\theta = \mathbf{l}/r$ and $\mathbf{l} = \mathbf{l}'$. Then, the convergence power spectrum defined by Eq. (8.100) reads

$$P_\kappa(l) = \left(\frac{3H_0^2 \Omega_m^{(0)}}{2} \right)^2 \int_0^\infty dr \left(\frac{g(r)}{a(r)} \right)^2 P_{\delta_{\text{eff}}}(l/r, r). \quad (8.105)$$

The power spectra of shear fields γ_1 and γ_2 can be computed in a similar way. Defining $\tilde{\kappa}(r') = -[\psi_{\text{eff},11}(r') + \psi_{\text{eff},22}(r')]/2$, $\tilde{\gamma}_1(r') = -[\psi_{\text{eff},11}(r') - \psi_{\text{eff},22}(r')]/2$,

$\tilde{\gamma}_2(r') = -\psi_{\text{eff},12}(r')$ in Eqs. (8.92)–(8.94), the corresponding values in the two-dimensional Fourier space are given, respectively, by $\tilde{\kappa}(\mathbf{l}) = (l^2/2)\psi(l)$, $\tilde{\gamma}_1(\mathbf{l}) = (l_1^2 - l_2^2)\psi(l)/2$, $\tilde{\gamma}_2(\mathbf{l}) = l_1 l_2 \psi(l)$, where l_1 and l_2 are components of the vector field $\mathbf{l}$ along the θ^1 and θ^2 axes, respectively. Introducing the angle φ_l between $\mathbf{l}$ and the θ^1 axis, it follows that $l_1 = l \cos \varphi_l$ and $l_2 = l \sin \varphi_l$. Hence we obtain

$$\tilde{\gamma}_1(\mathbf{l}) = \tilde{\kappa}(l) \cos(2\varphi_l), \quad \tilde{\gamma}_2(\mathbf{l}) = \tilde{\kappa}(l) \sin(2\varphi_l). \quad (8.106)$$

Then, the power spectra $P_{\gamma_1}(\mathbf{l})$ and $P_{\gamma_2}(\mathbf{l})$ of shear fields γ_1 and γ_2 are related to $P_\kappa(l)$ as

$$P_{\gamma_1}(\mathbf{l}) = P_\kappa(l) \cos^2(2\varphi_l), \quad P_{\gamma_2}(\mathbf{l}) = P_\kappa(l) \sin^2(2\varphi_l). \quad (8.107)$$

Defining the cross power spectra $P_{\gamma_1\gamma_2}(\mathbf{l})$ of γ_1 and γ_2 as $\langle \gamma_1(\mathbf{l}) \gamma_2^*(\mathbf{l}') \rangle = (2\pi)^2 \delta^{(2)}(\mathbf{l} - \mathbf{l}')$, it follows that

$$P_{\gamma_1\gamma_2}(\mathbf{l}) = P_\kappa(l) \cos(2\varphi_l) \sin(2\varphi_l). \quad (8.108)$$

Unlike $P_\kappa(l)$, the power spectra of shear fields depend not only on the amplitude of $\mathbf{l}$ but also on its direction. In other words, the power spectra like $P_{\gamma_1}(\mathbf{l})$ depend on the choice of the two-dimensional coordinate (θ^1, θ^2) . To remove this dependence, we consider a coordinate transformation under which the θ^1 axis is rotated with the angle φ . Then, the matrix A defined by Eq. (8.91) is transformed as

$$\hat{A} = C A C^{-1}, \quad C = \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix}. \quad (8.109)$$

The convergence field is invariant under this coordinate transformation ($\hat{\kappa} = \kappa$), but the shear fields are transformed as $\hat{\gamma}_1 = \gamma_1 \cos(2\varphi) + \gamma_2 \sin(2\varphi)$ and $\hat{\gamma}_2 = -\gamma_1 \sin(2\varphi) + \gamma_2 \cos(2\varphi)$. After rotating the θ^1 axis, its direction coincides with that of the vector $\mathbf{l}$ by choosing $\varphi = \varphi_l$. Writing the transformed values of $\hat{\gamma}_1$ and $\hat{\gamma}_2$ as E and B , respectively, it follows that

$$\begin{pmatrix} E(\mathbf{l}) \\ B(\mathbf{l}) \end{pmatrix} = \begin{pmatrix} \cos(2\varphi_l) & \sin(2\varphi_l) \\ -\sin(2\varphi_l) & \cos(2\varphi_l) \end{pmatrix} \begin{pmatrix} \gamma_1(\mathbf{l}) \\ \gamma_2(\mathbf{l}) \end{pmatrix}, \quad (8.110)$$

where $E(\mathbf{l})$ and $B(\mathbf{l})$ are called the E-mode and the B-mode, respectively. The E-mode quantifies the distortion parallel to the wavenumber $\mathbf{l}$ or orthogonal to $\mathbf{l}$. The B-mode characterizes the distortion along the direction inclined by the angle $\pi/4$ from the direction of $\mathbf{l}$.

Substituting Eq. (8.106) into Eq. (8.110), we obtain $\tilde{E}(\mathbf{l}) = \tilde{\kappa}(l)$ and $\tilde{B}(\mathbf{l}) = 0$, i.e., the vanishing B-mode. After the coordinate transformation, the power spectra of the E-mode, the B-mode, and their cross correlations are given, respectively, by

$$P_E(l) = P_\kappa(l), \quad P_B(l) = 0, \quad P_{EB}(l) = 0, \quad (8.111)$$

which correspond to setting $\varphi_l = 0$ in Eqs. (8.107) and (8.108). Hence only the E-mode, which is attributed to the convergence field, remains as the physical degree

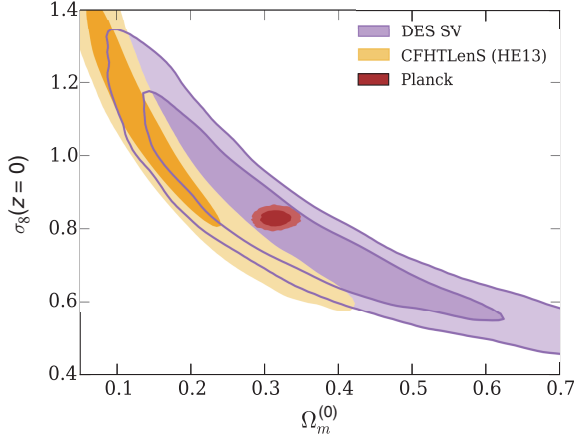


Fig. 8.9. Constraints on $\sigma_8(z=0)$ and today's matter density $\Omega_m^{(0)}$ from DES SV cosmic shear [33], CFHTLenS [34], and Planck 2015 [12] measurements. We show 68% CL and 95% CL observational contours in the flat Λ CDM model. Reproduced from Ref. [33].

of freedom. From Eqs. (8.92)–(8.94), the quantities κ , γ_1 , γ_2 are generated by the scalar gravitational potential ψ_{eff} , so there is no rotational degree of freedom. This is the reason why the B-mode is not generated by the weak gravitational lensing.

From Eq. (8.105), the convergence power spectrum is related to the power spectrum $P_{\delta_{\text{eff}}}$ of the effective density field, so the observations of $P_{\kappa}(l)$ provide the information of the matter power spectrum. In Fig. 8.9, we show constraints on $\sigma_8(z=0)$ and $\Omega_m^{(0)}$ derived from two weak lensing measurements: (a) Dark Energy Survey Science Verification (DES SV) [33], and (b) Canada–France–Hawaii Telescope Legacy Survey (CFHTLenS) [34]. The DES SV data are consistent with the Planck bounds on $\sigma_8(z=0)$ and $\Omega_m^{(0)}$, while the CFHTLenS data are in some tension with the Planck measurement. The observations of weak lensing have not been precise enough to place tight bounds on the property of dark energy (like the equation of state w_{DE}), but the accuracy of measurements will be improved in the future.

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Chapter 9

Cosmological Constant

The cosmological constant Λ is the simplest model of dark energy. However, if it originates from the vacuum energy, its predicted energy scale is vastly larger than the observed dark energy scale. Since the existence of such large values of Λ spoils the known expansion history of the Universe, the cosmological constant problem was recognized as a serious problem even before the discovery of the late-time cosmic acceleration in 1998 [1]. In this chapter, we first review the fine-tuning problem of Λ by explicitly calculating the vacuum energy and present a number of approaches that aim to tackle this problem.¹

9.1. Cosmological constant problem

The Einstein equation with the cosmological constant Λ is given by Eq. (3.86), so the energy-momentum tensor corresponding to Λ reads

$$T_{\mu\nu}^{(\Lambda)} = -\Lambda M_{\text{pl}}^2 g_{\mu\nu}, \quad (9.1)$$

where $M_{\text{pl}} = (8\pi G)^{-1/2}$ is the reduced Planck mass, and we used the unit $c = 1$. The component $T_{00}^{(\Lambda)}$ corresponds to the energy density ρ_Λ with $g_{00} = -1$ on the FLRW background (4.1), so that $\rho_\Lambda = \Lambda M_{\text{pl}}^2$. If the energy density ρ_Λ is much larger than the today's average energy density $\rho_0 \approx M_{\text{pl}}^2 H_0^2$ of the Universe, then the cosmic expansion history has been spoiled. On using the fact that H_0 is of the order of 10^{-42} GeV, Weinberg derived the following bound in 1987 [11]:

$$-10^{-47} \text{ GeV}^4 \lesssim \rho_\Lambda \lesssim 3 \times 10^{-45} \text{ GeV}^4. \quad (9.2)$$

The upper bound is attributed to the requirement that the vacuum energy did not dominate over matter densities at redshifts $z \gtrsim \mathcal{O}(1)$. The lower bound comes

¹Due to the diversity of the problem, there are other approaches to the cosmological constant problem which are not addressed in this book. Readers may have a look at the references [2–10] for further interests.

from the condition that ρ_Λ does not cancel the today's cosmological density. If the cosmological constant is responsible for the present acceleration, the energy density ρ_Λ should be of the order

$$\rho_\Lambda \approx M_{\text{pl}}^2 H_0^2 \approx 10^{-47} \text{ GeV}^4. \quad (9.3)$$

This can be interpreted as the mass scale $m_\Lambda = \rho_\Lambda^{1/4} \sim 1 \text{ meV}$.

On the other hand, the energy-momentum tensor $T_{\mu\nu}$ of a field in the vacuum state is given by the expectation value

$$\langle T_{\mu\nu} \rangle \equiv \langle 0 | T_{\mu\nu} | 0 \rangle = -\rho_{\text{vac}} g_{\mu\nu}, \quad (9.4)$$

where ρ_{vac} is the constant energy density of vacuum. If we consider a canonical scalar field ϕ with the potential $V(\phi)$, the energy-momentum tensor is given by Eq. (4.93). The vacuum corresponds to the energy state at which the scalar field sits at the minimum of its potential with the field value ϕ_{min} . In this vacuum state the field kinetic energy vanishes in Eq. (4.93), so the covariant energy-momentum tensor of vacuum becomes

$$\langle T_{\mu\nu} \rangle = -V(\phi_{\text{vac}}) g_{\mu\nu}, \quad (9.5)$$

so that $\rho_{\text{vac}} = V(\phi_{\text{vac}})$ as expected.

If the cosmological constant originates from the vacuum energy, then we require that ρ_{vac} is in the range

$$|\rho_{\text{vac}}| \lesssim M_{\text{pl}}^2 H_0^2 \approx 10^{-47} \text{ GeV}^4. \quad (9.6)$$

In Sec. 9.2, we will show that the vacuum energy density ρ_{vac} computed in quantum field theory receives contributions of the fourth power of a mass term m . If we consider electrons with mass $m_e \simeq 0.5 \text{ MeV}$, this contribution can be estimated as $\rho_{\text{vac}} \sim m_e^4 \sim 10^{-13} \text{ GeV}^4$, which is 10^{34} times as large as ρ_Λ given by Eq. (9.3). Hence the electron already gives rise to too much vacuum energy. Since heavier particles exist at least up to the electroweak scale ($\sim \text{TeV}$), the vacuum energies associated with them are larger than that of electrons.

As we will see in Sec. 9.2, the one-loop vacuum energy density ρ_{vac} contains a divergent term, which can be regulated by adding a counter-term ρ_c to absorb the divergence. Then, the renormalized vacuum energy density is given by

$$\rho_{\text{re}} = \rho_{\text{vac}} + \rho_c. \quad (9.7)$$

Let us consider the vacuum energy associated with a particle with mass m of the order of TeV . From observations we require that $|\rho_{\text{re}}| \lesssim (\text{meV})^4$, but ρ_{vac} contains the contribution $m^4 \sim 10^{60} (\text{meV})^4$. Hence we need to cancel two big numbers to realize a tiny value of $|\rho_{\text{re}}|$. This is generally known as the cosmological constant problem [12, 13].

Historically, the real serious consideration about the cosmological constant started after the success of the idea of spontaneous symmetry breaking into the

electroweak theory [14–16]. The electroweak phase transition in the early Universe leads to a jump of the vacuum energy of the order of $\Delta V_{\text{EW}} \sim (200 \text{ GeV})^4$. Even if we could adjust the vacuum energy to be small before (after) the phase transition, it would show up after (before) the transition. The similar situation also arises for the QCD phase transition with a jump $\Delta V_{\text{QCD}} \sim (0.3 \text{ GeV})^4$. The cosmological constant problem is attributed to the fact that the mass scale m_Λ associated with dark energy is too small compared to typical mass scales of elementary particles.

9.2. Vacuum energy and fine tuning at quantum level

We compute the vacuum energy of a free scalar field ϕ with mass m on the Minkowski background with the metric $\eta_{\mu\nu}$. The Lagrangian density of such a scalar field is given by

$$\mathcal{L} = -\frac{1}{2}\eta^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - \frac{1}{2}m^2\phi^2, \quad (9.8)$$

where $\partial_\mu\phi \equiv \partial\phi/\partial x^\mu$. Varying this Lagrangian density with respect to ϕ , we obtain the Klein–Gordon equation

$$-\ddot{\phi} + \delta^{ij}\partial_i\partial_j\phi - m^2\phi = 0. \quad (9.9)$$

From Eq. (4.92), the energy–momentum tensor of ϕ is

$$T_{\mu\nu} = \partial_\mu\phi\partial_\nu\phi - \eta_{\mu\nu}\left[\frac{1}{2}\partial^\alpha\phi\partial_\alpha\phi + V(\phi)\right]. \quad (9.10)$$

The energy density measured by a rest-frame observer with the four-velocity $u^\mu = (1, 0, 0, 0)$ is given by $\rho = u^\mu u^\nu T_{\mu\nu} = T_{00}$, which leads to

$$\rho = \frac{1}{2}\dot{\phi}^2 + \frac{1}{2}(\partial\phi)^2 + \frac{1}{2}m^2\phi^2, \quad (9.11)$$

where $(\partial\phi)^2 \equiv \delta^{ij}\partial_i\phi\partial_j\phi$. Similarly, the pressure measured by the observer can be computed from $P = (\eta^{\mu\nu} + u^\mu u^\nu)T_{\mu\nu}/3$, such that

$$P = \frac{1}{2}\dot{\phi}^2 - \frac{1}{6}(\partial\phi)^2 - \frac{1}{2}m^2\phi^2. \quad (9.12)$$

To compute the vacuum expectation values of ρ and P , we expand the scalar field in Fourier series according to the standard prescription of quantum field theory [17] as

$$\phi(t, \mathbf{x}) = \frac{1}{(2\pi)^3} \int \frac{d^3\mathbf{k}}{\sqrt{2\omega}} [a(\mathbf{k})e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} + a^\dagger(\mathbf{k})e^{i\omega t - i\mathbf{k}\cdot\mathbf{x}}], \quad (9.13)$$

where ω is the temporal component of the four momentum $k^\mu = (k^0, \mathbf{k})$, i.e., $\omega = k^0$. Since the scalar field obeys Eq. (9.9), there is the relation $\omega = \sqrt{k^2 + m^2}$ with $k = |\mathbf{k}|$. The coefficients $a(\mathbf{k})$ and $a^\dagger(\mathbf{k})$ are quantum operators (annihilation and creation operators, respectively) obeying the commutation

relations (6.160) and (6.161). The vacuum expectation values of the quantities $\dot{\phi}^2$, $(\partial\phi)^2$, $m^2\phi^2$ in Eqs. (9.11) and (9.12) can be easily computed as [12]

$$\langle 0|\dot{\phi}^2|0\rangle = \frac{1}{(2\pi)^3} \int \frac{d^3\mathbf{k}}{2\omega} \omega^2, \quad (9.14)$$

$$\langle 0|(\partial\phi)^2|0\rangle = \frac{1}{(2\pi)^3} \int \frac{d^3\mathbf{k}}{2\omega} k^2, \quad (9.15)$$

$$\langle 0|m^2\phi^2|0\rangle = \frac{1}{(2\pi)^3} \int \frac{d^3\mathbf{k}}{2\omega} m^2. \quad (9.16)$$

Then, the vacuum expectation values of ρ and P are given, respectively by

$$\langle \rho \rangle = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\omega}{2}, \quad (9.17)$$

$$\langle P \rangle = \frac{1}{3} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{k^2}{2\omega}. \quad (9.18)$$

Since both $\langle \rho \rangle$ and $\langle P \rangle$ are divergent, one usually introduces a ultra-violet cut-off Λ_{UV} for the computations of integrals. Performing the expansion in terms of the small parameter $\epsilon = m/\Lambda_{\text{UV}}$, it follows that [18]

$$\begin{aligned} \langle \rho \rangle &= \int_0^{\Lambda_{\text{UV}}} \frac{dk}{4\pi^2} k^2 \sqrt{k^2 + m^2} \\ &= \frac{\Lambda_{\text{UV}}^4}{16\pi^2} + \frac{m^2 \Lambda_{\text{UV}}^2}{16\pi^2} + \frac{m^4}{64\pi^2} \ln \left(\frac{m^2 e^{1/2}}{4\Lambda_{\text{UV}}^2} \right) + \mathcal{O}(\Lambda_{\text{UV}}^{-2}), \end{aligned} \quad (9.19)$$

$$\begin{aligned} \langle P \rangle &= \frac{1}{3} \int_0^{\Lambda_{\text{UV}}} \frac{dk}{4\pi^2} \frac{k^4}{\sqrt{k^2 + m^2}} \\ &= \frac{\Lambda_{\text{UV}}^4}{48\pi^2} - \frac{m^2 \Lambda_{\text{UV}}^2}{48\pi^2} - \frac{m^4}{64\pi^2} \ln \left(\frac{m^2 e^{7/6}}{4\Lambda_{\text{UV}}^2} \right) + \mathcal{O}(\Lambda_{\text{UV}}^{-2}). \end{aligned} \quad (9.20)$$

In most of the literature, the first term on the right hand side of Eq. (9.19), which diverges in the limit $\Lambda_{\text{UV}} \rightarrow \infty$, is not removed to derive a renormalized expression of the vacuum energy. Taking the Planck scale $m_{\text{pl}} \simeq 10^{19}$ GeV as a natural cut-off scale for Λ_{UV} (in the sense that perturbative calculations in quantum field theory are trustable), it follows that $\langle \rho \rangle_{\text{UV}} \simeq \Lambda_{\text{UV}}^4/(16\pi^2) \simeq 10^{74}$ GeV⁴. The usual statement of the cosmological constant problem is that this value is different from the observed value (9.6) by 121 order of magnitude. This argument assumes that the cut-off should not be sent to infinity, so the vacuum energy depends on the choice of cut-off. Moreover, as we will see below, this vacuum state does not respect the Lorentz symmetry.

From experiments, we know that the quantum vacuum is Lorentz invariant with high accuracy [19], so the vacuum energy-momentum tensor $T_{\mu\nu}$ on the Minkowski

background should be of the form (9.4). This means that the expectation values of ρ and P should satisfy [18, 20]

$$\langle \rho \rangle = -\langle P \rangle. \quad (9.21)$$

The dominant contribution to the pressure (9.20) in the ultra-violet regime is given by $\langle P_{UV} \rangle = \Lambda_{UV}^4 / (48\pi^2)$. Since this is related to $\langle \rho \rangle_{UV}$ as $\langle P_{UV} \rangle = \langle \rho \rangle_{UV} / 3$, it does not obey the property (9.21). The second terms on the right hand side of Eqs. (9.19) and (9.20), which diverge in the limit $\Lambda_{UV} \rightarrow \infty$, do not have the property (9.21) either.

The divergences of $\langle \rho \rangle$ and $\langle P \rangle$ should be regulated in such a way that the vacuum state respects the Lorentz symmetry. It is possible to eliminate the first two Lorentz-violating terms in Eqs. (9.20) and (9.21) by adding local counter-terms. We can also introduce a renormalization scale μ to eliminate logarithmic divergences in the third terms of Eqs. (9.19) and (9.20). Absorbing remaining numerical factors to respect the Lorentz symmetry, the resulting renormalized vacuum energy becomes

$$\langle \rho \rangle_{\text{ren}} = -\langle P \rangle_{\text{ren}} = \frac{m^4}{64\pi^2} \ln \left(\frac{m^2}{\mu^2} \right). \quad (9.22)$$

There are other contributions to the expansions (9.19) and (9.20) containing powers of mass m , but the logarithmic term derived above should be most physical in the sense that it cannot be eliminated by a local counter-term if the mass is generated by the Higgs mechanism.

The result same as Eq. (9.22) can be derived by using a so-called dimensional regularization [17]. This is a renormalization scheme respecting the Lorentz invariance formulated in a D -dimensional Minkowski spacetime. By extending Eqs. (9.17) and (9.18), we compute the following integrals

$$\langle \rho \rangle = \mu^{4-D} \int \frac{d^{D-1} \mathbf{k}}{(2\pi)^{D-1}} \frac{1}{2} \sqrt{k^2 + m^2}, \quad (9.23)$$

$$\langle P \rangle = \frac{\mu^{4-D}}{D-1} \int \frac{d^{D-1} \mathbf{k}}{(2\pi)^{D-1}} \frac{k^2}{2\sqrt{k^2 + m^2}}, \quad (9.24)$$

where we introduced a mass scale μ for the dimensional reason. We compute the integrals (9.23) and (9.24) in a dimension where they converge. Analytic continuation leads to the Lorentz-invariant vacuum energy [12, 18, 20]

$$\langle \rho \rangle = -\langle P \rangle = -\frac{\mu^4 \Gamma(-D/2)}{2^{D+1} \pi^{D/2}} \left(\frac{m}{\mu} \right)^D, \quad (9.25)$$

where $\Gamma(x)$ is the Gamma function that diverges at $x = -2$. To see the property of the divergence at $D = 4$, we set $D = 4 - \epsilon$ and expand Eq. (9.25) in terms of the small parameter ϵ . In doing so, we use the fact that the Gamma function is expanded as $\Gamma(-2 + \epsilon/2) = 1/\epsilon + 3/4 - \gamma_E/2 + \mathcal{O}(\epsilon)$, where $\gamma_E \simeq 0.5772$ is the

Euler–Mascheroni constant. In the limit $\epsilon \rightarrow 0$, the vacuum energy (9.25) can be expressed as

$$\langle \rho \rangle = -\langle P \rangle = \frac{m^4}{64\pi^2} \left[-\frac{2}{\epsilon} + \gamma_E - \frac{3}{2} + \ln \left(\frac{m^2}{4\pi\mu^2} \right) \right], \quad (9.26)$$

which matches with the calculation using one loop diagram for the scalar field ϕ [17]. Employing a minimal subtraction scheme removing the pole $-1/\epsilon$, the renormalized vacuum energy yields

$$\langle \rho \rangle_{\text{ren}} = -\langle P \rangle_{\text{ren}} = \frac{m^4}{64\pi^2} \left[\gamma_E - \frac{3}{2} + \ln \left(\frac{m^2}{4\pi\mu^2} \right) \right]. \quad (9.27)$$

If we further use a non-minimal scheme of regulation subtracting the contributions $\gamma_E, -3/2, -\ln(4\pi)$ in the square bracket of Eq. (9.27), then the renormalized vacuum energy fully agrees with Eq. (9.22).

For massless particles the renormalized vacuum energy (9.22) vanishes, but for massive particles it depends on the renormalization scale μ . The sign of $\langle \rho \rangle_{\text{ren}}$ is positive (or negative) for $\mu < m$ (or for $\mu > m$). Since μ is an unknown mass scale, we cannot predict the concrete value of $\langle \rho \rangle_{\text{ren}}$ itself. More importantly, the finite contributions of the order of m^4 , which appear on the right hand side of Eq. (9.27), need to be cancelled to an accuracy of the order of 10^{60} for the mass up to the TeV scale to address the cosmological constant problem.

So far we have switched off gravity, but all forms of energy including the vacuum energy affects the geometry of spacetime, i.e., the vacuum energy gravitates. In terms of the action principle, the vacuum energy V_{vac} couples to gravity with the covariant measure $S_{\text{vac}} = -\int d^4x \sqrt{-g} V_{\text{vac}}$. As we already discussed in Sec. 3.4, varying this action with respect to $g_{\mu\nu}$ and using the property (3.95), the vacuum energy contributes to the Einstein equation in the form $V_{\text{vac}} g_{\mu\nu}$.

In terms of Feynman diagrams there are vacuum loops connected to external graviton fields. In addition to the one-loop vacuum energy computed above, there are also two loops with external graviton legs. The two-loop correction to the vacuum energy scales are like λm^4 , where λ is a dimensionless coupling associated with the particle theory under consideration (e.g., $\lambda \sim 0.1$ for the Higgs field). Hence the two-loop correction is not necessarily small relative to the one-loop vacuum energy. This means that, even if the cancellation is imposed to obtain a tiny vacuum energy at the one-loop level, we need to tune two-loop contributions again with similar accuracy. The same property also persists for higher-order loops, so there is a problem of radiative instability where the fine tuning is repeatedly required at each perturbative order to extreme accuracy. This is the quantum-mechanical cosmological constant problem [13]. In other words, the tuning of the vacuum energy consistent with observations is fragile against any modification in the perturbative effective field theory.

9.3. Supersymmetric theories

There are several approaches to tackling the cosmological constant problem.² One of them is based on supersymmetric theories in which an exchanging symmetry between bosons and fermions is present. In the presence of supersymmetry down to the TeV scale, a large hierarchy problem between the Planck scale (10^{19} GeV) and the electroweak scale (10^2 GeV) can be addressed in such a way that the Higgs particle does not receive huge masses from quantum corrections. The question is whether supersymmetric theories can allow a vanishing or a very tiny vacuum energy consistent with observations.

In supersymmetric theories, there exists a quantum generator Q_s exchanging the spins between bosonic and fermionic states, as $Q_s|\text{boson}\rangle = |\text{fermion}\rangle$ and $Q_s|\text{fermion}\rangle = |\text{boson}\rangle$. For two-component spin indices a and b , the supersymmetric generators Q_a and $Q_b^\dagger$ obey the anti-commutation relation [21]

$$\{Q_a, Q_b^\dagger\} \equiv Q_a Q_b^\dagger + Q_b^\dagger Q_a = (\sigma_\mu)_{ab} P^\mu, \quad (9.28)$$

where $\sigma_0 = 1$, $\sigma_{1,2,3}$ are the Pauli matrices, and P^μ is the energy-momentum four-vector operator. Supersymmetry is unbroken under the conditions

$$Q_s|0\rangle = 0, \quad Q_s^\dagger|0\rangle = 0, \quad (9.29)$$

for all Q_s . From Eqs. (9.28) and (9.29), the vacuum expectation value of P^μ yields $\langle 0|P^\mu|0\rangle = 0$, so the vacuum energy vanishes.

This vanishing vacuum energy is the outcome of a globally supersymmetric theory without coupling to gravity [22]. The same result also follows from the potential of chiral scalar fields ϕ^i (where $i = 1, 2, \dots, N$) in the global supersymmetric theory:

$$V = \sum_{i=1}^N |W_{,\phi^i}|^2, \quad (9.30)$$

where $W(\phi^i, \phi^{i*})$ is the so-called superpotential with the notation $W_{,\phi^i} \equiv \partial W / \partial \phi^i$. Supersymmetry is unbroken for the superpotential stationary for all ϕ^i , in which case the vanishing vacuum energy ($V = 0$) follows from Eq. (9.30). However we know that supersymmetry is broken in the real world, so Eq. (9.30) gives rise to a non-vanishing vacuum energy.

In the presence of gravity, any globally supersymmetric theory is promoted to a locally supersymmetric supergravity theory. In supergravity theory, the vacuum energy is attributed to an expectation value of the potential V for chiral scalar fields

²The approaches given in Secs. 9.3 and 9.4 deal with advanced topics, so the reader who are not interested in these topics can skip these sections.

ϕ^i , which is given by [23–25]

$$V(\phi, \phi^*) = e^{K/M_{\text{pl}}^2} \left[D_i W (K^{ij*}) (D_j W)^* - \frac{3|W|^2}{M_{\text{pl}}^2} \right], \quad (9.31)$$

where K is called the Kähler potential that depends on ϕ^i and ϕ^{i*} , and K^{ij*} is the inverse of the quantity

$$K_{ij*} \equiv K_{,\phi^i \phi^{j*}}. \quad (9.32)$$

The derivative $D_i W$ is defined by

$$D_i W \equiv W_{,\phi^i} + \frac{W}{M_{\text{pl}}^2} K_{,\phi^i}. \quad (9.33)$$

The four-dimensional effective action in supergravity is expressed as

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} R - K_{ij*} \partial_\mu \phi^i \partial^\mu \phi^{j*} - V(\phi, \phi^*) \right], \quad (9.34)$$

where the second term corresponds to the kinetic term of chiral scalar fields. The condition for unbroken supersymmetry is $D_i W = 0$ for all i . This corresponds to an anti-de Sitter (AdS) minimum with the negative potential energy $V_{\text{AdS}} = -3e^{K/M_{\text{pl}}^2} |W|^2 / M_{\text{pl}}^2$. To realize a vanishing vacuum energy with unbroken supersymmetry, we require another condition $W = 0$.

If supersymmetry is broken ($D_i W \neq 0$), the first term in the square bracket of Eq. (9.31) contributes to the total potential energy. It is known that there exists a class of Kähler potentials and superpotentials that gives rise to the field configuration with $V = 0$. Let us consider two types of chiral scalar fields T and S with the Kähler potential [26]

$$K(T, S) = -3M_{\text{pl}}^2 \ln(T + T^*) - M_{\text{pl}}^2 \ln(S + S^*), \quad (9.35)$$

and the superpotential depending on the field S only

$$W = W(S). \quad (9.36)$$

For these functions, there is the relation

$$(D_T W) K^{TT*} (D_T W)^* - \frac{3|W|^2}{M_{\text{pl}}^2} = 0. \quad (9.37)$$

Hence the second term in the square bracket of Eq. (9.31) is cancelled by the contribution from the fields T . Then the resulting potential energy is given by

$$V = \frac{1}{(T + T^*)^3 (S + S^*)} (D_S W) K^{SS*} (D_S W)^*. \quad (9.38)$$

The kinetic Lagrangian density $\mathcal{L}_{\text{kin}} = -K_{ij*} \partial_\mu \phi^i \partial^\mu \phi^{j*}$ can be written in a canonical form $\mathcal{L}_{\text{kin}} = -\partial_\mu \tilde{T} \partial^\mu \tilde{T} / 2 - \partial_\mu \tilde{S} \partial^\mu \tilde{S} / 2$ by redefining $\tilde{T} = \sqrt{3/2} M_{\text{pl}} \ln T$ and $\tilde{S} = \sqrt{1/2} M_{\text{pl}} \ln S$.

From Eq. (9.38), it follows that the stationary field configuration with $V = 0$ can be realized at a field value S satisfying

$$D_S W = W_{,S} - \frac{W}{S + S^*} = 0. \quad (9.39)$$

Meanwhile, the derivative term $D_T W = -3W/(T + T^*)$ does not vanish for $W \neq 0$, in which case supersymmetry is broken. This means that the vanishing vacuum energy can be realized even with broken supersymmetry. While the field S is fixed at the value determined by Eq. (9.39), the field T is undetermined. The latter field appears only for the overall scale of the potential. These theories are called no-scale models [27].

The Kähler potential (9.35) and the superpotential (9.36) can arise in superstring theories after the compactification of six extra dimensions in ten-dimensional theories [28, 29] (see also the books [30, 31] for the introduction to string theories). In such cases, the scale of extra dimensions is quantified by a so-called modulus field T . We also have four-dimensional complex scalar fields S^i known as dilaton/axion fields. In a gluino condensation model studied in Ref. [28], the Kähler potential is of the form (9.35) with the factor 3 arising from the compactification on a complex manifold with $(10 - 4)/2 = 3$ complex dimensions. There are also gauge fields coupled to S but not to T . After integrating out gauge fields, the effective superpotential for S reduces to the form $W(S) = M_{\text{pl}}^3 [c_1 + c_2 \exp(-3S/2c_3)]$, where c_1, c_2, c_3 are constants. In such models it is possible to realize a non-supersymmetric field configuration with a vanishing vacuum energy.

Although these results are intriguing, the forms of Kähler potential (9.35) and superpotential (9.36) are the outcomes of lowest-order perturbation theory. It is expected that they should lose their validity beyond lowest-order perturbation theory, in such a way that the field potential is subject to a non-vanishing energy contribution [1]. This situation is similar to what we discussed in Sec. 9.2. Even if we were able to cancel the vacuum energy at lowest order, we encounter the problem that higher-order contributions spoil its success. Moreover, even if the vacuum energy were cancelled at all finite orders of perturbative theory, non-perturbative effects such as QCD instantons can give rise to a large contribution to the vacuum energy. This means that the perturbative theory at finite order is not generally sufficient to address the cosmological constant problem.

9.4. de Sitter vacua in string theory

In string theory, there is a no-go theorem by Gibbons [32] and Maldacena and Nunez [33] stating that, for an extra dimensional space with a time-independent

non-singular compact manifold without a boundary, a scalar field with a positive potential does not arise in the lowest-order effective string action. This no-go theorem is not valid in the presence of extended objects like branes [34] or higher-order corrections to the leading-order action, so there is the possibility for realizing de Sitter (dS) vacua in string theory.

In string theory, a string can be either open or closed. The end point of strings is required to lie on a p -dimensional dynamical object, which is called a p -brane [34]. A p -brane, which sweeps out a $(p+1)$ -dimensional volume in spacetime (called world-volume) has a mass and a charge. In string theory, there is a two-brane (membrane) with a charge q . Since the two-brane runs over the $(2+1)$ -dimensional volume, it sources a four-form field $F_{\mu\nu\lambda\sigma}$ associated with a three-form potential $A_{\nu\lambda\sigma}$, as [35]

$$F_{\mu\nu\lambda\sigma} = \partial_{[\mu} A_{\nu\lambda\sigma]}, \quad (9.40)$$

where the square bracket represents the total anti-symmetrization. This is analogous to the two-form Maxwell field $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ sourced by a point particle with charge q . Unlike two-branes, the charged point particle moves along a one-dimensional worldvolume.

In the absence of sources, the equation of motion for the four-form field $F^{\mu\nu\lambda\sigma}$ is given by $\partial_\mu(\sqrt{-g}F^{\mu\nu\lambda\sigma}) = 0$. This has the following solution:

$$F^{\mu\nu\lambda\sigma} = c \varepsilon^{\mu\nu\lambda\sigma}, \quad (9.41)$$

where c is a constant, and $\varepsilon^{\mu\nu\lambda\sigma}$ is the totally anti-symmetric Levi-Civita tensor defined by

$$\varepsilon_{\mu\nu\lambda\sigma} = \sqrt{-g} \bar{\varepsilon}_{\mu\nu\lambda\sigma}, \quad (9.42)$$

where $\bar{\varepsilon}_{\mu\nu\lambda\sigma} = 1$ for an even permutation of the subscript $(0, 1, 2, 3)$, $\bar{\varepsilon}_{\mu\nu\lambda\sigma} = -1$ for an odd permutation of the subscript $(0, 1, 2, 3)$, and $\bar{\varepsilon}_{\mu\nu\lambda\sigma} = 0$ for other cases. The Levi-Civita tensor satisfies the normalization $\varepsilon^{\mu\nu\lambda\sigma} \varepsilon_{\mu\nu\lambda\sigma} = -4!$. Then, the energy density arising from the four-form field yields

$$U(F) = -\frac{1}{2 \cdot 4!} F^{\mu\nu\lambda\sigma} F_{\mu\nu\lambda\sigma} = \frac{c^2}{2}. \quad (9.43)$$

The idea of making the cosmological constant variable in terms of the four-form energy density was originally advocated by Linde [36] and Brown and Teitelboim [37, 38] in the context of quantum creation of the Universe. Suppose that there is a scalar field ϕ with the potential energy $V(\phi)$ in addition to the four-form field with the energy density (9.43). Most probably, the Universe is created with the total energy density $\rho = V(\phi) + U(F)$ of the order of m_{pl}^4 . After the field ϕ roll downs to the potential minimum at $\phi = \phi_0$, the total effective cosmological constant is given by

$$\rho_{\text{eff}} = \rho_b + \frac{c^2}{2}, \quad (9.44)$$

where $\rho_b = V(\phi_0)$. The resulting value of ρ_{eff} is different depending on $V(\phi)$ and $U(F)$. In the early 1980s, the possibility for the creation of many mini-Universes separated from each other was discussed in the context of inflationary cosmology [39] (see also Ref. [40]). Among many possible values of ρ_{eff} , there exists at least a probability that the four-form energy density $c^2/2$ almost cancels the vacuum energy ρ_b . For this to happen, we require that ρ_b is negative. Linde argued that we may live in a vacuum with a tiny vacuum energy due to the anthropic selection from many other possible vacua [36].

In string theory, the constant c appearing in Eq. (9.41) can be quantized in integer multiples of the membrane charge q , as $c = nq$, where n is an integer [41]. In the presence of the vacuum energy ρ_b , the total effective cosmological constant (9.44) becomes

$$\rho_{\text{eff}} = \rho_b + \frac{n^2 q^2}{2}. \quad (9.45)$$

The difference of this from Eq. (9.44) is that the constant c is discrete after the quantization. In the presence of the negative vacuum energy ($\rho_b < 0$), we discuss the possibility for realizing a small value of ρ_{eff} . Analogous to the creation of an electron and a positron out of the vacuum, the membranes can be spontaneously created by a quantum tunneling effect. Since this leads to the discharge of the four-form field strength, i.e., $nq \rightarrow (n-1)q$, the energy density of the four-form field decreases by an amount

$$-\delta U = \left[\frac{1}{2} n^2 q^2 - \frac{1}{2} (n-1)^2 q^2 \right] = \left(n - \frac{1}{2} \right) q^2. \quad (9.46)$$

To realize the smallest value of ρ_{eff} in Eq. (9.45), the flux integer n_0 should be taken with a value nearest to $\sqrt{2|\rho_b|/q^2}$. In this case, the step size near $\rho_{\text{eff}} = 0$ is given by $(n_0 - 1/2)q^2 \simeq \sqrt{|\rho_b|q^2}$. The effective cosmological constant of the order of $\rho_{\text{eff}} \simeq 10^{-47} \text{ GeV}^4 \simeq 10^{-123} m_{\text{pl}}^4$ can be realized for

$$|q| \lesssim 10^{-123} |\rho_b|^{-1/2}, \quad (9.47)$$

in Planck units ($m_{\text{pl}} = 1$). The very small charge $|q|$ like Eq. (9.47) does not naturally arise in the context of string theory.

This problem of the small charge can be circumvented by taking into account the J number of four-form fields and membrane species with charges $q_1, q_2, \dots, q_J$ [41]. In string theory it is natural to consider the configuration with J of the order of 100. Since the i th four-form field strength is given by $F_i^{\mu\nu\lambda\sigma} = c_i \epsilon^{\mu\nu\lambda\sigma}$ with $c_i = n_i q_i$, the effective vacuum energy becomes

$$\rho_{\text{eff}} = \rho_b + \frac{1}{2} \sum_{i=1}^J n_i^2 q_i^2. \quad (9.48)$$

If there is a set of integers n_i satisfying

$$2|\rho_b| < \sum_{i=1}^J n_i^2 q_i^2 < 2(|\rho_b| + \Delta\rho), \quad (9.49)$$

with $\Delta\rho \simeq 10^{-123}$, then it is possible to realize ρ_{eff} of the same order as $\Delta\rho$. We take J -dimensional grids with each axis labelled by $n_i q_i$, where the four-form field is displaced at discrete grid points. The region (9.49) is characterized by a thin-shell with radius $r = \sqrt{|2\rho_b|}$ and width $\Delta r = \Delta\rho/\sqrt{|2\rho_b|}$. The thin-shell has the volume

$$V_s = \Omega_{J-1} r^{J-1} \Delta r = \Omega_{J-1} |2\rho_b|^{J/2-1} \Delta\rho, \quad (9.50)$$

where $\Omega_{J-1} = 2\pi^{J/2}/\Gamma(J/2)$ is the area of a unit $J-1$ dimensional sphere. The volume V_c of a grid cell is given by $V_c = \prod_{i=1}^J |q_i|$. Provided that $V_c < V_s$, i.e.,

$$\prod_{i=1}^J |q_i| < \frac{2\pi^{J/2}}{\Gamma(J/2)} |2\rho_b|^{J/2-1} \Delta\rho, \quad (9.51)$$

there is at least one value of ρ_{eff} . For $J = 100$, $|\rho_b| = 1$ and $\Delta\rho = 10^{-123}$ with equal charges ($q_i = q$, for $i = 1, 2, \dots, J$), the condition (9.51) is satisfied for $|q| < 0.035$. In terms of the unit of mass this translates to $\sqrt{|q|} < 0.19 m_{\text{pl}}$, so the natural charge can be allowed in the set-up of J four-form fields.

In string theory, there are in general six-dimensional compactified manifolds associated with the existence of extra dimensions. They have hundreds of different non-contractible three-spheres embedded in the compact manifold called three-cycles [35]. A five-brane, which can be viewed as a two-brane to a macroscopic observer, wraps any of these three-cycles. This gives rise to hundreds of different membranes in four-dimensional spacetime. The charges q_i are determined by the five-brane charge, the volume of compactified manifolds, and the three-cycle volume. In general the charges q_i are slightly smaller than unity, so this is consistent with the discussion given above.

So far we considered a simple scenario for the realization of a small effective cosmological constant in string theory, but the problem of the stabilization of extra dimensions should be also addressed in more realistic models. In 2003, Kachru, Kallosh, Linde and Trivedi (KKLT) [42] constructed de Sitter solutions compactified on a Calabi–Yau manifold in the presence of a flux. In the KKLT scenario, the first step is to stabilize all moduli fields (associated with the size of extra dimensions) at a supersymmetric AdS vacuum under the flux compactification. The second step is to add a small number of the anti-D3-brane in a warped geometry with a throat by breaking supersymmetry. This uplifts the AdS minimum to the dS vacuum without violating the stability of moduli fields.

In the flux compactification used in the KKLT scenario there can be 500 three-cycles with each cycle wrapped by up to 10 fluxes, which leads to 10^{500} vacua. The fact that a huge number of de Sitter vacua can arise in string theory led to the notion

of string landscape [43]. Our Universe may correspond to at least one of all possible de Sitter vacua in the landscape. The argument is that it should be statistically possible to find a vacuum with a very tiny energy density $10^{-123}m_{\text{pl}}^4$ among 10^{500} vacua. In this way, the string landscape is associated with the anthropic selection of vacua. Each vacuum has different matter and coupling constant, so the standard model of particle physics is not uniquely predicted in this picture.

However, it is not a very encouraging situation that string theory, which was originally supposed to make concrete predictions of physical constants in Nature in terms of a single string parameter, has not been able to predict a concrete value of the effective cosmological constant without resorting to the landscape statistics associated with the anthropic principle. The completion of string theory as a unified theory is still on the way, so its future development may improve the current situation.

9.5. Sequestering vacuum energy

There is an interesting mechanism proposed by Kaloper and Padilla for sequestering the vacuum energy from gravity [44–46]. There are two versions of the vacuum energy sequestering: (i) non-local theory and (ii) local theory.

The non-local version is based on two variables without having any local degrees of freedom: the bare cosmological constant Λ and the dimensionless scaling parameter λ fixing the hierarchy between matter-sector dimensional scales and the Planck mass. The cosmological constant is promoted to a global dynamical variable in such a way that it can be varied over in the action. The scaling global dynamical variable λ is introduced to realize a protected matter sector with a suppressed vacuum energy. The two variables Λ and λ talk to one another through a global interaction σ whose form is set by the dimensional analysis. In the non-local vacuum energy sequestering, this global term is not integrated over spacetime.

The local version is formulated by the existence of an integral that contains the product of a local term $\sigma(x)$ and an auxiliary four-form field $F_{\mu\nu\lambda\sigma}$ [47]. In the following, we first review how the sequestering mechanism works in the non-local version and then proceed to the resulting cosmological dynamics in the presence of a scalar field triggering the collapse of the Universe [46]. Finally, we discuss the local theory of vacuum energy sequestering in which the Universe can have an infinite volume.

9.5.1. Non-local theory of vacuum energy sequestering

We begin with the action [44, 45]

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} R + \lambda^4 \mathcal{L}_m(\lambda^{-2} g^{\mu\nu}, \Psi_m) - \Lambda \right] + \sigma \left(\frac{\Lambda}{\lambda^4 \mu^4} \right), \quad (9.52)$$

where $\mathcal{L}_m$ is the Lagrangian density of matter fields Ψ_m (including Standard Model particles), and μ is some mass scale associated with the quantum field theory cut-off. The global interaction $\sigma(\Lambda/(\lambda^4\mu^4))$, which is odd and differentiable, is not integrated over. Since this term is not an additive integral over spacetime, the vacuum energy sequestering scenario described by the action (9.52) is non-local.

The vacuum energy contributions arising from the matter Lagrangian $\sqrt{-g}\lambda^4\mathcal{L}_m(\lambda^{-2}g^{\mu\nu}, \Psi_m)$ have the scale dependence proportional to λ^4 . Introducing the rescaled metric

$$\hat{g}^{\mu\nu} = \lambda^{-2}g^{\mu\nu}, \quad (9.53)$$

the matter Lagrangian is expressed as

$$\sqrt{-g}\lambda^4\mathcal{L}_m(\lambda^{-2}g^{\mu\nu}, \Psi_m) = \sqrt{-\hat{g}}\mathcal{L}_m(\hat{g}^{\mu\nu}, \Psi_m), \quad (9.54)$$

where we used the property $\sqrt{-\hat{g}} = \sqrt{-g}\lambda^4$. Hence the parameter λ corresponds to a rescaling factor between the “Jordan frame” metric $\hat{g}^{\mu\nu}$ and the “Einstein frame” metric $g^{\mu\nu}$. As we see in the action (9.52), the reduced Planck mass M_{Pl} is fixed in the Einstein frame, while the mass m scales as $m = \lambda\hat{m}$, where $\hat{m}$ is the mass that appears in the Lagrangian density $\mathcal{L}_m$.

The energy–momentum tensors in the “Jordan frame” and the “Einstein frame” are given, respectively, by

$$\hat{T}_{\mu\nu} = -\frac{2}{\sqrt{-\hat{g}}}\frac{\delta}{\delta\hat{g}^{\mu\nu}}\left(\sqrt{-\hat{g}}\mathcal{L}_m(\hat{g}^{\mu\nu}, \Psi_m)\right), \quad (9.55)$$

$$T_{\mu\nu} = -\frac{2}{\sqrt{-g}}\frac{\delta}{\delta g^{\mu\nu}}\left(\sqrt{-g}\lambda^4\mathcal{L}_m(\hat{g}^{\mu\nu}, \Psi_m)\right) = \lambda^2\hat{T}_{\mu\nu}. \quad (9.56)$$

The trace $\hat{T}_\mu^\mu = \hat{g}^{\mu\nu}\hat{T}_{\mu\nu}$ is

$$\hat{T}_\mu^\mu = 4\mathcal{L}_m - 2\hat{g}^{\mu\nu}\frac{\delta\mathcal{L}_m}{\delta\hat{g}^{\mu\nu}}, \quad (9.57)$$

which is related to $T_\mu^\mu = g^{\mu\nu}T_{\mu\nu}$, as $T_\mu^\mu = \lambda^4\hat{T}_\mu^\mu$.

Varying the action (9.52) with respect to Λ and λ , it follows that

$$\frac{1}{\lambda^4\mu^4}\sigma'(y) = \int d^4x\sqrt{-g}, \quad (9.58)$$

$$\frac{4\Lambda}{\lambda^4\mu^4}\sigma'(y) = \int d^4x\sqrt{-g}T_\mu^\mu, \quad (9.59)$$

respectively, where $y = \Lambda/(\lambda^4\mu^4)$ and $\sigma'(y) = d\sigma/dy$. Eliminating the term $\sigma'(y)$ from Eqs. (9.58) and (9.59), we obtain

$$\Lambda = \frac{1}{4}\langle T_\mu^\mu \rangle, \quad (9.60)$$

where $\langle T_\mu^\mu \rangle$ is the spacetime average of T_μ^μ defined by

$$\langle T_\mu^\mu \rangle \equiv \frac{\int d^4x \sqrt{-g} T_\mu^\mu}{\int d^4x \sqrt{-g}}. \quad (9.61)$$

Variation of the action (9.52) with respect to $g^{\mu\nu}$ leads to

$$\delta S = \int d^4x \sqrt{-g} \left(\frac{M_{\text{pl}}^2}{2} G_{\mu\nu} - \frac{1}{2} T_{\mu\nu} + \frac{1}{2} \Lambda g_{\mu\nu} \right) \delta g^{\mu\nu}. \quad (9.62)$$

Substituting the relation $\Lambda = \langle T_\alpha^\alpha \rangle / 4$ into Eq. (9.62), the gravitational equation becomes

$$M_{\text{pl}}^2 G_\nu^\mu = T_\nu^\mu - \frac{1}{4} \langle T_\alpha^\alpha \rangle \delta_\nu^\mu. \quad (9.63)$$

The matter energy-momentum tensor can be expressed in the form

$$T_\nu^\mu = -V_{\text{vac}} \delta_\nu^\mu + \tau_\nu^\mu, \quad (9.64)$$

where V_{vac} is the vacuum energy arising from the matter loops in Standard Model and τ_ν^μ are the energy-momentum tensor associated with local excitations about the vacuum. Substituting Eq. (9.64) into Eq. (9.63), we find that the contribution of vacuum energy drops out from gravity. The resulting gravitational equation reads

$$M_{\text{pl}}^2 G_\nu^\mu = \tau_\nu^\mu - \frac{1}{4} \langle \tau_\alpha^\alpha \rangle \delta_\nu^\mu, \quad (9.65)$$

which means that the gravitational dynamics is determined by the locally excited matter. The cancellation of the vacuum energy V_{vac} is attributed to the fact that the coupling λ is universal to all matters at any order in loops. Hence the sequestering mechanism allows us to avoid the problem of fine tunings at each order in loops mentioned in Sec. 9.2. From Eq. (9.65), the residual effective cosmological constant is given by

$$\Lambda_{\text{eff}} = \frac{1}{4} \langle \tau_\alpha^\alpha \rangle, \quad (9.66)$$

which is determined by the historic average of local matter excitations. This does not give rise to any dangerous radiative corrections to the zero-point vacuum energy. In Ref. [45], it was also shown that the contributions arising from cosmological phase transitions to the effective vacuum energy are suppressed to below the critical density of today's Universe.

9.5.2. Collapsing Universe in non-local theory of vacuum energy sequestering

Let us proceed to the discussion of cosmological dynamics in the non-local theory of vacuum energy sequestering discussed in Sec. 9.5.1. From Eq. (9.58), the volume integral $\int d^4x \sqrt{-g}$ needs to be finite, so the Universe should be closed. This means that the present cosmic expansion would be halted at some point in the future. For example, this happens for a scalar field ϕ with a linear potential:

$$V(\phi) = \hat{m}^3 \phi, \quad (9.67)$$

where $\hat{m}$ is some mass scale. After the field enters the region with negative $V(\phi)$, the Universe enters the collapsing stage. The protected matter Lagrangian density is given by

$$\lambda^4 \mathcal{L}_m(\lambda^{-2} g^{\mu\nu}, \Psi_m) = \lambda^4 \tilde{\mathcal{L}}_m(\lambda^{-2} g^{\mu\nu}, \Psi_m) - \frac{\lambda^2}{2} g^{\mu\nu} \nabla_\mu \phi \nabla_\nu \phi - \lambda^4 V(\phi), \quad (9.68)$$

where $\tilde{\mathcal{L}}_m$ contains the contributions from Standard Model fields and local excitations.

The physical mass scale m in the Einstein frame is controlled by the scaling parameter λ , as $m = \lambda \hat{m}$. Provided that the mass term m is sufficiently small, the linear potential (9.67) can drive the present (transient) cosmic acceleration. As we will see below, this happens for the mass scale of the order of $m \simeq (M_{\text{pl}} H_0^2)^{1/3}$. In general, such a tiny mass can be spoiled by radiative corrections. For the linear potential (9.67), however, there is a mechanism for protecting the small mass against radiative corrections. Under the shift $\phi \rightarrow \phi + \mathcal{C}$, the full matter Lagrangian density changes as $\mathcal{L}_m \rightarrow \mathcal{L}_m - \hat{m}^3 \mathcal{C}$. This is absorbed by the shift of the global variable $\Lambda \rightarrow \Lambda - \lambda^4 \hat{m}^3 \mathcal{C}$, under which the integral part of the action (9.52) is invariant. The shift of Λ induces the changes of the variable $y = \Lambda/(\lambda^4 \mu^4)$ by an amount $-\hat{m}^3 \mathcal{C}/\mu^4$. Provided that the cut-off scale μ is sufficiently large, say $\mu \sim M_{\text{pl}}$, and the mass $\hat{m}$ is as small as that required for the late-time cosmic acceleration, it follows that $\hat{m}^3 \mathcal{C}/\mu^4 \ll 1$. Hence there exists the approximate shift symmetry that protects the linear potential (9.67) against radiative corrections [46].

Introducing a canonical scalar field $\varphi = \lambda \phi$, the field Lagrangian density on the right hand side of Eq. (9.68) can be expressed in the form $\mathcal{L}_\phi = -g^{\mu\nu} \nabla_\mu \varphi \nabla_\nu \varphi / 2 - m^3 \varphi$. Then, the energy-momentum tensor of matter fields can be expressed as

$$\tau_\nu^\mu = \tilde{\tau}_\nu^\mu + \nabla^\mu \varphi \nabla_\nu \varphi - \delta_\nu^\mu \left(\frac{1}{2} \nabla^\alpha \varphi \nabla_\alpha \varphi + m^3 \varphi \right), \quad (9.69)$$

where $\tilde{\tau}_\nu^\mu$ is the contribution to τ_ν^μ other than φ . The historic average of τ_μ^μ is given by $\langle \tau_\mu^\mu \rangle = \langle \tilde{\tau}_\mu^\mu \rangle - \langle \nabla^\alpha \varphi \nabla_\alpha \varphi \rangle - 4m^3 \langle \varphi \rangle$. Under the shift $\varphi \rightarrow \varphi + \tilde{\mathcal{C}}$, the trace $\langle \tau_\mu^\mu \rangle$

is transformed as

$$\langle \tau_\mu^\mu \rangle \rightarrow \langle \tau_\mu^\mu \rangle - 4m^3 \tilde{\mathcal{C}}. \quad (9.70)$$

This means that $\langle \tau_\mu^\mu \rangle$ can take any arbitrary value by shifting the origin of φ . In particular, we can choose the “gauge” satisfying the constraint

$$\langle \tau_\mu^\mu \rangle = 0. \quad (9.71)$$

In the following, we study the cosmological dynamics for the potential $m^3\varphi$ with initial conditions respecting the gauge condition (9.71). Taking into account matter whose energy density ρ and the pressure P obey the continuity equation $\dot{\rho} + 3H(\rho + P) = 0$, the constraint (9.71) translates to

$$\langle 3P - \rho \rangle + \langle \dot{\varphi}^2 \rangle - 4m^3 \langle \varphi \rangle = 0. \quad (9.72)$$

On the closed FLRW background in which the spatial curvature $\mathcal{K}$ is positive, the gravitational equations (9.65) give

$$3M_{\text{pl}}^2 \left(H^2 + \frac{\mathcal{K}}{a^2} \right) = \rho + \frac{1}{2} \dot{\varphi}^2 + m^3 \varphi, \quad (9.73)$$

$$2M_{\text{pl}}^2 \left(\dot{H} - \frac{\mathcal{K}}{a^2} \right) = -\rho - P - \dot{\varphi}^2. \quad (9.74)$$

The scalar field φ obeys the equation of motion

$$\ddot{\varphi} + 3H\dot{\varphi} + m^3 = 0. \quad (9.75)$$

If the mass scale m is of the order of $m \simeq (M_{\text{pl}} H_0^2)^{1/3}$, the Universe expands by the time $t_0 \sim H_0^{-1}$ and exhibits a short stage of acceleration before the collapse starts. In the early Universe during which the field density is much smaller than the background matter density (radiation or non-relativistic matter), the scale factor grows as $a \propto t^p$ with $p > 0$. Integrating Eq. (9.75) after the substitution of $H = p/t$ and neglecting the decaying mode, the evolution of φ is given by

$$\varphi \simeq \varphi_0 - \frac{m^3 t^2}{2(3p+1)} = \varphi_0 - \frac{m^3}{2(3p+1)} \left(\frac{p}{H} \right)^2, \quad (9.76)$$

where φ_0 is a constant. The estimation (9.76) is valid by the time t_1 at which the background density becomes the same order as the field density, i.e., $\rho(t_1) \approx m^3 \varphi_1$, where φ_1 is the field value at $t = t_1$. The field variation from the initial value φ_{in} (Hubble parameter H_{in}) to the value φ_1 (Hubble parameter H_1) can be estimated as

$$\varphi_1 - \varphi_{\text{in}} = -\mathcal{O}(1) \frac{m^3}{H_1^2}, \quad (9.77)$$

where we used the approximation $H_{\text{in}} \gg H_1$. For $m^3 \simeq M_{\text{pl}} H_0^2$ and $H_0 < H_1$, the field variation $\varphi_{\text{in}} - \varphi_1$ is smaller than the order of M_{pl} .

For $t > t_1$, the field density starts to dominate over the background matter density. There is a transient stage of cosmic acceleration during which the field evolves slowly along the linear potential in the region $V > 0$. In this regime the slow-roll conditions $\dot{\varphi}^2/2 \ll m^3\varphi$ and $|\ddot{\varphi}| \ll |3H\dot{\varphi}|$ are satisfied, so Eqs. (9.73) and (9.75) approximately read

$$3M_{\text{pl}}^2 H^2 \simeq m^3\varphi, \quad 3H\dot{\varphi} \simeq -m^3, \quad (9.78)$$

where we ignored the spatial curvature term $\mathcal{K}$. Eliminating the Hubble parameter H from these equations, it follows that

$$\dot{\varphi} \simeq -\frac{M_{\text{pl}} m^{3/2}}{\sqrt{3}\varphi^{1/2}}. \quad (9.79)$$

The slow-roll parameter defined by $\epsilon \equiv \dot{\varphi}^2/(2m^3\varphi)$ reduces to $\epsilon \simeq M_{\text{pl}}^2/(6\varphi^2)$. The slow-roll period ends when φ drops below M_{pl} . From Eq. (9.79), we obtain the integrated solution

$$\frac{2}{3}\varphi^{3/2} \simeq -\frac{m^{3/2}}{\sqrt{3}}M_{\text{pl}}(t - t_1) + \frac{2}{3}\varphi_1^{3/2}. \quad (9.80)$$

The time t_2 at which the slow-roll period ends can be estimated as

$$t_2 \simeq t_1 + \mathcal{O}(1)\sqrt{\frac{M_{\text{pl}}}{m^3}}. \quad (9.81)$$

For $t > t_2$, the scalar field rapidly rolls down the potential to enter the region with $m^3\varphi < 0$. The time t_3 at turnover, which is identified by the condition $\dot{\varphi}^2/2 \simeq -m^3\varphi$, is of the same order as t_2 , i.e., $t_3 \simeq t_1 + \mathcal{O}(1)\sqrt{M_{\text{pl}}/m^3}$. Since the Universe collapses after the turnover, the total age of the Universe can be estimated as $t_3 \sim 1/H_3$, where H_3 is the Hubble parameter at turnover. The spacetime volume $\int d^4x\sqrt{-g}$ has a finite maximum size of the order of $1/H_3^3$.

We recall that there is the constraint (9.72) that restricts the initial condition of φ . Reflecting the fact that the Universe is spatially compact and collapses, the left hand side of Eq. (9.72) is dominated by the contributions around the turnover, such that $\langle 3P - \rho \rangle \simeq -\mathcal{O}(1)M_{\text{pl}}^2 H_3^2$ and $\langle \dot{\varphi}^2 \rangle - 4m^3\langle \varphi \rangle \simeq -\mathcal{O}(1)m^3\varphi(t_3)$. Then, the field value at turnover can be estimated as

$$\varphi(t_3) \simeq -\mathcal{O}(1)\frac{M_{\text{pl}}^2 H_3^2}{m^3} \simeq -\mathcal{O}(1)\left(\frac{H_3}{H_0}\right)^2 M_{\text{pl}} \lesssim -M_{\text{pl}}. \quad (9.82)$$

We have already seen that the slow-roll cosmic acceleration occurs in the regime $\varphi \gtrsim M_{\text{pl}}$ during the time interval $t_1 < t < t_2$. Taking into account the condition (9.82), the field variation larger than M_{pl} occurs for $t_2 < t < t_3$. From the initial time t_{in} to t_1 , the variation of the field remains sub-Planckian. This argument shows that the initial field value is in the range

$$\varphi_{\text{in}} \gtrsim M_{\text{pl}}, \quad (9.83)$$

under which the Universe undergoes the temporal accelerating stage and then finally enters the collapsing phase.

The constraint (9.71) is not generally satisfied for arbitrary initial conditions. For the success of the vacuum energy sequestering, we require that $\langle \tau_\mu^\mu \rangle$ is at most of the order of the present cosmological density ρ_0 . For the linear potential (9.67), we have shown that the sequestering mechanism can be at work for initial conditions satisfying Eq. (9.83). We caution that the quantity $\langle \tau_\mu^\mu \rangle$ is the spacetime average, so it depends on the whole cosmological evolution including the future. While we have estimated $\langle \tau_\mu^\mu \rangle$ by picking up the contribution around turnover as the main source, the strict calculation for this quantity requires the integration from the Big Bang to the end of the cosmic evolution. This means that, unless we solve the dynamical equations of motion by the end (including from today to future), the *present* value of $\langle \tau_\mu^\mu \rangle$ is unknown. Numerically, we can confirm that there are initial conditions in the range (9.83) that allow $\langle \tau_\mu^\mu \rangle$ smaller than the order of ρ_0 , in which case the sequestering mechanism is at work.

9.5.3. Local theory of vacuum energy sequestering

The global term $\sigma(\Lambda/(\lambda^4\mu^4))$ is not an additive integral over spacetime, so the sequestering scenario discussed so far is non-local. Existence of the non-local term is apparently in conflict with the microscopic origin of the mechanism. From the viewpoint of quantum field theory, the local theory containing additive integrals (like Feynman path integrals) looks more promising. In fact, it is possible to construct a manifestly local theory of vacuum energy sequestering by introducing integrals that contain auxiliary four-form fields [47].

In the action (9.52) of the non-local theory of vacuum energy sequestering, there are two rigid parameters λ and Λ without having any local degrees of freedom. For the computational simplicity, we first transform the “Einstein frame” action (9.52) to the “Jordan frame” action under the rescaling (9.53) of the metric. In doing so, we use the transformation laws $\sqrt{-g} = \lambda^{-4}\sqrt{-\hat{g}}$, $R = \lambda^2\hat{R}$, and Eq. (9.54). Defining the variables $\kappa^2 = M_{\text{pl}}^2/\lambda^2$ and $\hat{\Lambda} = \Lambda/\lambda^4$, the Jordan frame action reads

$$S_{\text{NL}} = \int d^4x \sqrt{-\hat{g}} \left[\frac{\kappa^2}{2} \hat{R} + \mathcal{L}_m(\hat{g}^{\mu\nu}, \Psi_m) - \hat{\Lambda} \right] + \sigma \left(\frac{\hat{\Lambda}}{\mu^4} \right), \quad (9.84)$$

which contains two rigid variables κ^2 and $\hat{\Lambda}$ instead of λ and Λ . In the non-local sequestering scenario, the quantities κ^2 and Λ are independent of the spacetime point x , but now we would like to promote these variables to local fields $\kappa^2(x)$ and $\Lambda(x)$ with additive integrals. These local fields should not gravitate to maintain the success of vacuum energy sequestering in the non-local version.

For this purpose, we resort to the fact that the covariant volume element $\sqrt{-g}d^4x$ can be expressed in the form

$$\sqrt{-g}d^4x = \frac{1}{4!} \varepsilon_{\mu\nu\lambda\sigma} dx^\mu dx^\nu dx^\lambda dx^\sigma, \quad (9.85)$$

where $\varepsilon_{\mu\nu\lambda\sigma}$ is the Levi-Civita tensor defined by Eq. (9.42). For the construction of a manifestly local action allowing the sequestering mechanism, we first consider the action containing a four-form field $F_{\mu\nu\lambda\sigma}$ written in terms of the measure analogous to the right hand side of Eq. (9.85):

$$S_F = - \int \Lambda(x) \left(\sqrt{-g} d^4x - \frac{1}{4!} F_{\mu\nu\lambda\sigma} dx^\mu dx^\nu dx^\lambda dx^\sigma \right), \quad (9.86)$$

where $F_{\mu\nu\lambda\sigma}$ is expressed in terms of the three-form potential $A_{\nu\lambda\sigma}$, as $F_{\mu\nu\lambda\sigma} = \partial_{[\mu} A_{\nu\lambda\sigma]}$. Varying the action (9.86) with respect to $\Lambda(x)$ gives $F_{\mu\nu\lambda\sigma} = \varepsilon_{\mu\nu\lambda\sigma}$, so $F_{\mu\nu\lambda\sigma}$ is a non-dynamical auxiliary field. Since the field $F_{\mu\nu\lambda\sigma}$ in the action (9.86) is independent of the metric, it does not appear in the gravitational equations of motion. The variation of Eq. (9.86) with respect to $A_{\nu\lambda\sigma}$ leads to $\partial_\mu \Lambda(x) = 0$, so the Lagrange multiplier $\Lambda(x)$ is an arbitrary constant. Hence the action (9.86), which is local and additive, does not give rise to any propagating degrees of freedom.

The same non-dynamical properties of $F_{\mu\nu\lambda\sigma}$ and Λ also persist by replacing the term $\varepsilon_{\mu\nu\lambda\sigma} dx^\mu dx^\nu dx^\lambda dx^\sigma / 4!$ in the action (9.86) with a more general function $\sigma(\Lambda/\mu^4) \varepsilon_{\mu\nu\lambda\sigma} dx^\mu dx^\nu dx^\lambda dx^\sigma / 4!$ multiplied by $\sigma(\Lambda/\mu^4)$. Since we have another local variable $\kappa^2(x)$, we can introduce the integral $\int \tilde{\sigma}(\kappa^2(x)/M_{\text{pl}}^2) \tilde{F}_{\mu\nu\lambda\sigma} dx^\mu dx^\nu dx^\lambda dx^\sigma / 4!$ to make κ^2 local off shell and constant on shell, where $\tilde{\sigma}$ is a function of the dimensionless ratio $\kappa^2(x)/M_{\text{pl}}^2$ and $\tilde{F}_{\mu\nu\lambda\sigma} = \partial_{[\mu} \tilde{A}_{\nu\lambda\sigma]}$ is another four-form field. Then, the action of a local theory of vacuum energy sequestering is given by

$$S_L = \int d^4x \sqrt{-g} \left[\frac{\kappa^2(x)}{2} R + \mathcal{L}_m(g^{\mu\nu}, \Psi_m) - \Lambda(x) \right] \\ + \frac{1}{4!} \int dx^\mu dx^\nu dx^\lambda dx^\sigma \left[\sigma \left(\frac{\Lambda(x)}{\mu^4} \right) F_{\mu\nu\lambda\sigma} + \tilde{\sigma} \left(\frac{\kappa^2(x)}{M_{\text{pl}}^2} \right) \tilde{F}_{\mu\nu\lambda\sigma} \right], \quad (9.87)$$

where we omitted the hat for the quantities in the Jordan frame.

Varying the action (9.87) with respect to $\kappa^2(x)$, the resulting gravitational equation of motion yields

$$\kappa^2(x) G_\nu^\mu = (\nabla^\mu \nabla_\nu - \delta_\nu^\mu \nabla^2) \kappa^2(x) + T_\nu^\mu - \Lambda(x) \delta_\nu^\mu, \quad (9.88)$$

where $T_{\mu\nu}$ is the matter energy-momentum tensor in the Jordan frame. Variations of the action (9.87) with respect to $\Lambda(x)$, $\kappa(x)$, $A_{\nu\lambda\sigma}$, $\tilde{A}_{\nu\lambda\sigma}$ lead, respectively, to

$$\frac{\sigma'(y)}{\mu^4} F_{\mu\nu\lambda\sigma} = \varepsilon_{\mu\nu\lambda\sigma}, \quad \frac{\tilde{\sigma}'(z)}{M_{\text{pl}}^2} \tilde{F}_{\mu\nu\lambda\sigma} = -\frac{1}{2} R \varepsilon_{\mu\nu\lambda\sigma}, \quad (9.89)$$

$$\frac{\sigma'(y)}{\mu^4} \partial_\mu \Lambda(x) = 0, \quad \frac{\tilde{\sigma}'(z)}{M_{\text{pl}}^2} \partial_\mu \kappa^2(x) = 0, \quad (9.90)$$

where $y = \Lambda(x)/\mu^4$ and $z = \kappa^2(x)/M_{\text{pl}}^2$. From Eq. (9.90), both $\Lambda(x)$ and $\kappa^2(x)$ are constants. Unlike the non-local case, the above equations of motion do not contain the volume integral $\int d^4x \sqrt{-g}$, so the Universe does not need to be finite.

Taking the trace of Eq. (9.88) and averaging it over spacetime, we obtain the relation

$$\Lambda = \frac{1}{4}\langle T_\alpha^\alpha \rangle + \Delta\Lambda, \quad (9.91)$$

where $\Delta\Lambda$ can be derived by taking the average of Eq. (9.89), such that

$$\Delta\Lambda = \frac{1}{4}\kappa^2\langle R \rangle = -\frac{\mu^4}{2} \frac{\kappa^2}{M_{\text{pl}}^2} \frac{\tilde{\sigma}'(z)}{\sigma'(y)} \frac{\langle \tilde{F}_{\mu\nu\lambda\sigma} \rangle}{\langle F_{\mu\nu\lambda\sigma} \rangle}. \quad (9.92)$$

Substituting Eq. (9.91) into Eq. (9.88), the gravitational equation yields

$$\kappa^2 G_\nu^\mu = T_\nu^\mu - \frac{1}{4}\langle T_\alpha^\alpha \rangle \delta_\nu^\mu - \Delta\Lambda \delta_\nu^\mu. \quad (9.93)$$

Expressing the matter energy-momentum tensor T_ν^μ in the form (9.64), the vacuum energy contribution $-V_{\text{vac}}\delta_\nu^\mu$ completely vanishes from the right hand side of Eq. (9.93), such that

$$\kappa^2 G_\nu^\mu = \tau_\nu^\mu - \frac{1}{4}\langle \tau_\alpha^\alpha \rangle \delta_\nu^\mu - \Delta\Lambda \delta_\nu^\mu. \quad (9.94)$$

Apart from the existence of the last term in Eq. (9.94), the vacuum energy sequestering works in the similar way to that in the non-local case.

The residual cosmological constant $\Delta\Lambda$ in Eq. (9.94) is determined by the ratios of two four-form fluxes and derivatives of the functions $\tilde{\sigma}(z)$ and $\sigma(y)$. The ratio $\langle \tilde{F}_{\mu\nu\lambda\sigma} \rangle / \langle F_{\mu\nu\lambda\sigma} \rangle = \int d^4x \sqrt{-g} \tilde{F}_{\mu\nu\lambda\sigma} / \int d^4x \sqrt{-g} F_{\mu\nu\lambda\sigma}$ should be integrated over the whole region of the locally Lorentzian box. Hence the fluxes are infrared quantities associated with the box size, i.e., insensitive to the ultra-violet cut-off. The loop corrections to $\tilde{F}_{\mu\nu\lambda\sigma}$ and $F_{\mu\nu\lambda\sigma}$ arise from the κ^2 and Λ dependences in the action (9.87). Provided that the dimensionless ratios κ^2/M_{pl}^2 and Λ/μ^4 are smaller than the order of 1, the variations of loop corrections are suppressed for smooth functions $\tilde{\sigma}(z)$ and $\sigma(y)$. Hence the residual cosmological constant is stable against radiation corrections.

The value of $\Delta\Lambda$ is not uniquely fixed by the underlying theory, but it should be measured to match with observations. To explain the present cosmic acceleration, it is fixed as $\Delta\Lambda \approx 10^{-12} \text{ eV}^4$. In this case, the Universe expands forever toward an infinite volume. Then the flux integrals $\int d^4x \sqrt{-g} \tilde{F}_{\mu\nu\lambda\sigma}$ and $\int d^4x \sqrt{-g} F_{\mu\nu\lambda\sigma}$ diverge, but as we see in Eq. (9.89), both $\tilde{F}_{\mu\nu\lambda\sigma}$ and $F_{\mu\nu\lambda\sigma}$ are finite in the Universe approaching a de Sitter solution. Hence the divergences of two flux integrals merely come from the volume factor $\int d^4x \sqrt{-g}$, so their ratio and $\Delta\Lambda$ remain finite. In Eq. (9.94), there exists the term $-\langle \tau_\alpha^\alpha \rangle \delta_\nu^\mu / 4$ arising from the local matter excitation. For the matter with a constant equation of state w larger than -1 , the spacetime average $\langle \tau_\alpha^\alpha \rangle$ has the scale-factor dependence $\langle \tau_\alpha^\alpha \rangle \propto a^{-3(1+w)}$, so it vanishes in the infinitely expanding Universe.

Thus we have shown that the local theory given by the action (9.87) allows the sequestering of vacuum energy generated by matter loops. The auxiliary four-form

fields play roles to cancel the vacuum energy, while leaving a radiative stable and finite contribution $\Delta\Lambda$ to the cosmological constant. The value of this finite contribution is theoretically arbitrary and it is bounded by cosmological measurements such that $\Delta\Lambda \lesssim 10^{-12} \text{ eV}^4$. If there are other matter sources in τ_ν^μ responsible for the present cosmic acceleration, the residual cosmological constant $\Delta\Lambda$ can be much smaller than 10^{-12} eV^4 . Taking $\kappa^2 = M_{\text{pl}}^2$ in the gravitational equation (9.94), the local theory of vacuum energy sequestering is equivalent to GR in the presence of a locally excited matter with a very tiny effective cosmological constant.

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Chapter 10

Modified Matter Models of Dark Energy

If the cosmological constant problem is solved in such a way that it vanishes (almost) completely, we need to find an alternative mechanism to explain today's cosmic acceleration. Broadly speaking, there are two approaches to addressing the dark energy problem. One of them is to introduce a specific form of matter with a negative pressure — which we call modified matter models. Another is known as modified gravity models in which the large-distance modification of gravity drives the cosmic acceleration. In this chapter, we review modified matter models of dark energy, paying particular attention to scalar-field models (quintessence and k-essence) and coupled dark energy with dark matter.

10.1. Quintessence

The simplest modified matter model of dark energy is called quintessence in which a canonical scalar field ϕ with a potential energy $V(\phi)$ leads to the acceleration of the Universe [1–7]. The mechanism of the cosmic acceleration is similar to slow-roll inflation discussed in Sec. 4.6, but the difference is that the energy density associated with the quintessence potential is much smaller than that of the inflaton potential. The scalar-field mass m_ϕ associated with dark energy is as light as the today's Hubble parameter $H_0 \simeq 10^{-33}$ eV. Such a ultra-light scalar field does not arise in Standard Model of particle physics. There were attempts to construct quintessence models in the framework of supergravity and string theories. In this section, we first review the basics of quintessence such as the dynamical system analysis and proceed to the classification of quintessence potentials in terms of the field equation of state. We then discuss the construction of particle physics models of quintessence.

10.1.1. Dynamical system

We consider the system of a canonical scalar field ϕ with a potential $V(\phi)$ and a matter perfect fluid. We are primarily interested in the case where the matter fluid is described by non-relativistic matter like CDM or baryon (i.e., after the onset of the matter-dominated epoch). If we identify the matter fluid as radiation, the discussion given below can be also applied to the radiation-dominated epoch in which the contribution of non-relativistic matter is negligible. The action under consideration is given by

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} R - \frac{1}{2} g^{\mu\nu} \nabla_\mu \phi \nabla_\nu \phi - V(\phi) \right] + S_m(g_{\mu\nu}, \Psi_m), \quad (10.1)$$

where S_m is the action of matter fields Ψ_m . We assume that the quintessence field ϕ does not have a direct coupling to matter fields.

On the flat FLRW background with the line element $ds^2 = -dt^2 + a^2(t) \cdot \delta_{ij} dx^i dx^j$, the energy density ρ_ϕ and the pressure P_ϕ of quintessence are given, respectively, by Eqs. (4.94) and (4.95). Then, the dark energy equation of state is

$$w_{\text{DE}} \equiv \frac{P_\phi}{\rho_\phi} = \frac{\dot{\phi}^2/2 - V(\phi)}{\dot{\phi}^2/2 + V(\phi)}. \quad (10.2)$$

The scalar-field equation of motion is given by Eq. (4.98), i.e.,

$$\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} = 0. \quad (10.3)$$

The barotropic matter fluid with the energy density ρ_m and the equation of state w_m obeys the continuity equation

$$\dot{\rho}_m + 3H(1 + w_m)\rho_m = 0. \quad (10.4)$$

For constant w_m , the matter energy density evolves as $\rho_m \propto a^{-3(1+w_m)}$.

On the flat FLRW background, the (00) and (11) components of Einstein equations are given, respectively, by Eqs. (4.15) and (4.16) with $\rho = \rho_\phi + \rho_m$, $P = P_\phi + w_m \rho_m$, and $\mathcal{K} = 0$. Then, we obtain

$$3M_{\text{pl}}^2 H^2 = \frac{1}{2} \dot{\phi}^2 + V(\phi) + \rho_m, \quad (10.5)$$

$$2M_{\text{pl}}^2 \dot{H} = -\dot{\phi}^2 - (1 + w_m)\rho_m. \quad (10.6)$$

To deal with the above dynamical system, it is convenient to introduce the following dimensionless variables:

$$x \equiv \frac{\dot{\phi}}{\sqrt{6}H M_{\text{pl}}}, \quad y \equiv \frac{\sqrt{V(\phi)}}{\sqrt{3}H M_{\text{pl}}}, \quad (10.7)$$

with which the dark energy equation of state (10.2) becomes

$$w_{\text{DE}} = \frac{x^2 - y^2}{x^2 + y^2}. \quad (10.8)$$

Hence the quintessence equation of state is in the range $w_{\text{DE}} \geq -1$. If we consider a phantom field where the kinetic energy of ϕ is given by $-\dot{\phi}^2/2$, it is possible to realize $w_{\text{DE}} < -1$ [8, 9]. However, it is known that such a ghost field gives rise to a catastrophic instability of the vacuum [10, 11]. Hence we focus on the quintessence field with a normal sign of the kinetic term.

We can express Eq. (10.5) in the form

$$\Omega_\phi + \Omega_m = 1, \quad (10.9)$$

where Ω_ϕ and Ω_m are the density parameters of quintessence and matter defined, respectively, by

$$\Omega_\phi \equiv \frac{\rho_\phi}{3M_{\text{pl}}^2 H^2} = x^2 + y^2, \quad \Omega_m \equiv \frac{\rho_m}{3M_{\text{pl}}^2 H^2}. \quad (10.10)$$

From Eq. (10.6), it follows that

$$\frac{\dot{H}}{H^2} = -3x^2 - \frac{3}{2}(1 + w_m)(1 - x^2 - y^2). \quad (10.11)$$

The effective equation of state $w_{\text{eff}} = -1 - 2\dot{H}/(3H^2)$ is

$$w_{\text{eff}} = w_m + (1 - w_m)x^2 - (1 + w_m)y^2. \quad (10.12)$$

Taking the derivatives of x and y with respect to $\mathcal{N} \equiv \ln a$ and using Eqs. (10.3) and (10.11), we obtain the dynamical equations of motion [12]

$$\frac{dx}{d\mathcal{N}} = -3x + \frac{\sqrt{6}}{2}\lambda y^2 + \frac{3}{2}x[(1 - w_m)x^2 + (1 + w_m)(1 - y^2)], \quad (10.13)$$

$$\frac{dy}{d\mathcal{N}} = -\frac{\sqrt{6}}{2}\lambda xy + \frac{3}{2}y[(1 - w_m)x^2 + (1 + w_m)(1 - y^2)], \quad (10.14)$$

where λ is defined by

$$\lambda \equiv -\frac{M_{\text{pl}} V_{,\phi}}{V}. \quad (10.15)$$

For constant λ , the above dynamical system reduces to an autonomous system, so the dynamics of dark energy is known by solving Eqs. (10.13) and (10.14). In Sec. 10.1.2, we first study the case in which λ is constant. After Sec. 10.1.3, we will address the case where λ varies in time.

Table 10.1. Fixed points for the exponential potential.

Name	x	y	Ω_ϕ	w_{eff}	w_{DE}
(a)	0	0	0	w_m	—
(b1)	1	0	1	1	1
(b2)	-1	0	1	1	1
(c)	$\frac{\lambda}{\sqrt{6}}$	$\sqrt{1 - \frac{\lambda^2}{6}}$	1	$-1 + \frac{\lambda^2}{3}$	$-1 + \frac{\lambda^2}{3}$
(d)	$\sqrt{\frac{3}{2}} \frac{1 + w_m}{\lambda}$	$\sqrt{\frac{3(1 - w_m^2)}{2\lambda^2}}$	$\frac{3(1 + w_m)}{\lambda^2}$	w_m	w_m

10.1.2. Exponential potentials

The model with constant λ corresponds to the exponential potential [6, 12, 13]

$$V(\phi) = V_0 e^{-\lambda\phi/M_{\text{pl}}}, \quad (10.16)$$

where V_0 is a constant. In this case, the fixed points of the autonomous system can be derived by setting $dx/d\mathcal{N} = 0$ and $dy/d\mathcal{N} = 0$ in Eqs. (10.13) and (10.14). In Table 10.1 we show the five fixed points and the corresponding values of $\Omega_\phi, w_{\text{eff}}, w_{\text{DE}}$.

Since $w_{\text{eff}} = 1$ for the points (b1) and (b2), they are irrelevant to radiation, matter, and accelerated epochs. For the non-relativistic matter fluid ($w_m = 0$), the matter-dominated epoch ($w_{\text{eff}} \simeq 0, \Omega_\phi \ll 1$) can be realized either by (a) or (d). The point (d) is known as the scaling solution [12] along which the ratio Ω_ϕ/Ω_m is a non-vanishing constant. For the realization of the matter-dominated epoch ($\Omega_m \simeq 1$) by the scaling solution, we require that $\lambda^2 \gg 1$. The point (c) can realize the cosmic acceleration ($w_{\text{eff}} < -1/3$) for $\lambda^2 < 2$. If we want the late-time cosmic acceleration, the transition from (d) to (c) is not possible. Instead, the system should evolve from (a) to (c) for $\lambda^2 < 2$. The radiation-dominated epoch corresponds to the fixed point (a) with the matter equation of state $w_m = 1/3$.

To study the stabilities of fixed points $(x, y) = (x_c, y_c)$, we consider small perturbations δx and δy around them. In general, the linear perturbations obey the differential equations

$$\frac{d}{d\mathcal{N}} \begin{pmatrix} \delta x \\ \delta y \end{pmatrix} = \mathcal{M} \begin{pmatrix} \delta x \\ \delta y \end{pmatrix}, \quad (10.17)$$

where the 2×2 matrix $\mathcal{M}$ is given by

$$\mathcal{M} = \begin{pmatrix} f_{1,x} & f_{1,y} \\ f_{2,x} & f_{2,y} \end{pmatrix}_{x=x_c, y=y_c}. \quad (10.18)$$

The functions $f_1(x, y)$ and $f_2(x, y)$ correspond to the right hand side of Eqs. (10.13) and (10.14), respectively, with the notation $f_{1,x} \equiv \partial f_1 / \partial x$. The components of the matrix $\mathcal{M}$ should be evaluated at each fixed point. If the two eigenvalues μ_1 and μ_2 of $\mathcal{M}$ are negative, the corresponding fixed point is a stable node. If one of the eigenvalues is negative and another is positive, the fixed point corresponds to a saddle. When both μ_1 and μ_2 are positive, the fixed point is unstable. If μ_1 and μ_2 are complex with negative real parts, the fixed point corresponds to a stable spiral.

The eigenvalues $\mathcal{M}$ of the five fixed points are given, respectively, by

$$\begin{aligned}
 \text{(a)} \quad & \mu_1 = -\frac{3}{2}(1 - w_m), \quad \mu_2 = \frac{3}{2}(1 + w_m). \\
 \text{(b1)} \quad & \mu_1 = 3 - \frac{\sqrt{6}\lambda}{2}, \quad \mu_2 = 3(1 - w_m). \\
 \text{(b2)} \quad & \mu_1 = 3 + \frac{\sqrt{6}\lambda}{2}, \quad \mu_2 = 3(1 - w_m). \\
 \text{(c)} \quad & \mu_1 = \frac{1}{2}(\lambda^2 - 6), \quad \mu_2 = \lambda^2 - 3(1 + w_m). \\
 \text{(d)} \quad & \mu_{1,2} = -\frac{3(1 - w_m)}{4} \left[1 \pm \sqrt{1 - \frac{8(1 + w_m)[\lambda^2 - 3(1 + w_m)]}{\lambda^2(1 - w_m)}} \right].
 \end{aligned}$$

For $0 \leq w_m \leq 1$ (which includes the case of both non-relativistic matter and radiation), the point (c) is stable for $\lambda^2 < 3(1 + w_m)$. The point (c) leads to the cosmic acceleration for $\lambda^2 < 2$, under which the same point is always stable. The point (a) is a saddle for $0 \leq w_m \leq 1$. This means that, for $\lambda^2 < 2$, the solutions eventually exit from the point (a) to approach the attractor point (c) with the cosmic acceleration. Note that the scaling point (d) is stable for $\lambda^2 > 3(1 + w_m)$ with the effective equation of state $w_{\text{eff}} = w_m$, but in this case the solution does not exit from the scaling matter era to give rise to the late-time acceleration.

Since both x and y are 0 at the point (a), w_{DE} is undetermined. In the realistic Universe, however, x and y are not exactly 0, such that the early evolution of w_{DE} depends on the initial conditions of x and y . If $x^2 \gg y^2$ and $x^2 \ll y^2$, then $w_{\text{DE}} \simeq 1$ and $w_{\text{DE}} \simeq -1$, respectively. Finally, the dark energy equation of state approaches the value $w_{\text{DE}} = -1 + \lambda^2/3$ of the fixed point (c). Since w_{DE} dynamically changes in time, the quintessence with the exponential potential can be observationally distinguished from the Λ CDM model.

10.1.3. General quintessence potentials

Except for the exponential potential, the slope λ defined by Eq. (10.15) depends on the field ϕ . Since Eqs. (10.13) and (10.14) are not closed in this case, we need to know the evolution of λ . However, it is still possible to derive analytic solutions to w_{DE} by classifying quintessence potentials according to the evolution of w_{DE} .

On using Eqs. (10.13) and (10.14) with Eqs. (10.9) and (10.11), we obtain the dynamical equations of the quantities w_{DE} and Ω_ϕ as

$$\frac{dw_{\text{DE}}}{d\mathcal{N}} = (w_{\text{DE}} - 1) \left[3(1 + w_{\text{DE}}) - \lambda \sqrt{3(1 + w_{\text{DE}})\Omega_\phi} \right], \quad (10.19)$$

$$\frac{d\Omega_\phi}{d\mathcal{N}} = -3(w_{\text{DE}} - w_m)\Omega_\phi(1 - \Omega_\phi). \quad (10.20)$$

The slope λ obeys the differential equation

$$\frac{d\lambda}{d\mathcal{N}} = -\sqrt{3(1 + w_{\text{DE}})\Omega_\phi}(\Gamma - 1)\lambda^2, \quad (10.21)$$

where

$$\Gamma \equiv \frac{VV_{,\phi\phi}}{V^2_{,\phi}}. \quad (10.22)$$

The evolution of w_{DE} is different depending on the forms of potentials and initial conditions of quintessence. Broadly speaking, we can classify quintessence potentials into three different classes: (i) tracking freezing models, (ii) scaling freezing models, and (iii) thawing models [14, 15]. In freezing models, the evolution of quintessence is fast in the early cosmological epoch, but it slows down at late times. Depending on the early evolution of w_{DE} , we can classify freezing models into the classes (i) and (ii). In thawing models (iii), the scalar field is nearly frozen during most of the cosmic expansion history, but it starts to evolve at late times.

10.1.3.1. Tracking freezing models

Let us consider the case in which the field density parameter obeys the relation

$$\Omega_\phi = \frac{3(1 + w_{\text{DE}})}{\lambda^2}. \quad (10.23)$$

Then, it follows from Eq. (10.19) that w_{DE} is constant. If $w_{\text{DE}} = w_m$, Eq. (10.20) shows that Ω_ϕ is constant and hence λ is constant for the solution (10.23). This corresponds to the scaling fixed point (d) given in Table 10.1. As we mentioned in Sec. 10.1.2, the scaling solution with constant λ is stable for $\lambda^2 > 3(1 + w_m)$, so it does not exit to the fixed point (c) relevant to dark energy.

If λ decreases in time, it is possible to enter the phase of cosmic acceleration. From Eq. (10.21), the condition for decreasing λ translates to

$$\Gamma > 1. \quad (10.24)$$

The solution (10.23) satisfying the condition (10.24) with nearly constant w_{DE} is dubbed a tracker [16, 17]. Along the tracker, the decrease of λ leads to the increase of Ω_ϕ , so w_{DE} is smaller than w_m from Eq. (10.20). The tracker is a common

evolutionary solution that attracts trajectories with different initial conditions. The solution (10.23) obeys the relation

$$\frac{\Omega'_\phi}{\Omega_\phi} = -\frac{2\lambda'}{\lambda}. \quad (10.25)$$

Substituting Eqs. (10.20) and (10.21) into Eq. (10.25) and using the approximation $\Omega_\phi \ll 1$ before the dark energy dominance, the field equation of state corresponding to the tracker is given by

$$w_{\text{DE}} = w_{(0)} \equiv \frac{w_m - 2(\Gamma - 1)}{2\Gamma - 1}. \quad (10.26)$$

Provided that Γ does not vary much, w_0 can be regarded as a constant.

As an example of the tracker solution, we consider the inverse power-law potential given by

$$V(\phi) = M^{4+p}\phi^{-p}, \quad (10.27)$$

where M and p (> 0) are constants. In this case, the quantity Γ is exactly constant, i.e., $\Gamma = 1 + 1/p$. As long as $p > 0$, the tracking condition (10.24) is automatically satisfied. The constant equation of state (10.26) reduces to [16, 17]

$$w_{(0)} = \frac{pw_m - 2}{p + 2}. \quad (10.28)$$

In the matter era ($w_m = 0$), it follows that $w_{(0)} = -2/(p + 2)$. For p closer to 0, $w_{(0)}$ approaches the value $w_{(0)} = -1$. Since the quantity λ defined by Eq. (10.15) is $\lambda = pM_{\text{pl}}/\phi$, the Universe enters the epoch of cosmic acceleration ($\lambda^2 < 2$) for

$$\phi > \frac{p}{\sqrt{2}}M_{\text{pl}}. \quad (10.29)$$

The equation of state (10.26) was derived under the approximation $\Omega_\phi \ll 1$. As Ω_ϕ grows, w_{DE} tends to deviate from the constant value $w_{(0)}$. In the presence of non-relativistic matter ($w_m = 0$), we estimate the variation of w_{DE} by dealing with Ω_ϕ as a perturbation δw to the zeroth-order solution (10.26), i.e., $w_{\text{DE}} = w_{(0)} + \delta w$. On using Eqs. (10.19) and (10.21) and assuming that Γ is nearly constant, the perturbation δw obeys [18]

$$a^2 \frac{d^2 \delta w}{da^2} + \frac{5 - 6w_{(0)}}{2} a \frac{d\delta w}{da} + \frac{9}{2} (1 - w_{(0)}) \delta w - \frac{9}{2} w_{(0)} (1 - w_{(0)}^2) \Omega_\phi(a) = 0, \quad (10.30)$$

up to linear order in δw . Substituting $w_{\text{DE}} = w_{(0)}$ into Eq. (10.20) and integrating it with respect to $\mathcal{N} = \ln a$, the zeroth-order solution to $\Omega_\phi(a)$ is given by $\Omega_\phi(a) =$

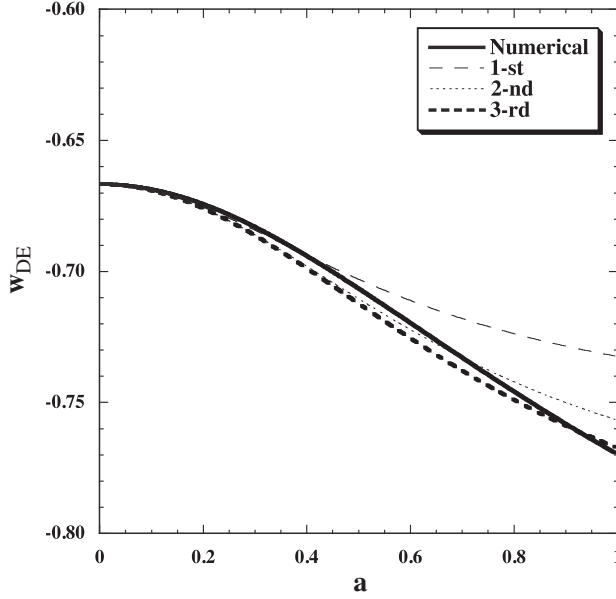


Fig. 10.1. The dark energy equation of state w_{DE} versus the scale factor a for the tracker solution realized by the inverse power-law potential $V(\phi) = M^5 \phi^{-1}$. The thick solid curve corresponds to the full numerical solution, whereas other three curves show the first, second, third order analytic solutions derived from Eq. (10.32).

$1/(1 + Ca^{3w_{(0)}})$. The integration constant C is fixed by using the field density parameter $\Omega_{\phi 0}$ today ($a = 1$), so the resulting zeroth-order solution is

$$\Omega_{\phi}(a) = \frac{\Omega_{\phi 0}}{\Omega_{\phi 0} + a^{3w_{(0)}}(1 - \Omega_{\phi 0})}. \quad (10.31)$$

Substituting Eq. (10.31) into Eq. (10.30), the integrated solution is given by [18]

$$w_{\text{DE}}(a) = w_{(0)} + \sum_{n=1}^{\infty} \frac{(-1)^{n-1} w_{(0)} (1 - w_{(0)}^2)}{1 - (n+1)w_{(0)} + 2n(n+1)w_{(0)}^2} \left(\frac{\Omega_{\phi}(a)}{1 - \Omega_{\phi}(a)} \right)^n. \quad (10.32)$$

In Fig. 10.1, we show the evolution of w_{DE} derived by using the analytic solution (10.32) for $p = 1$. The analytic estimation at third order is in fairly good agreement with the full numerical solution. The dark energy equation of state in the early matter era ($a < 0.1$) is nearly constant with the value close to $w_{(0)} = -2/3$. As Ω_{ϕ} increases, the decrease of w_{DE} starts to occur. Since the slope λ decreases toward 0, the solutions approach the “instantaneous” fixed point (c) with the time-varying equation of state $w_{\text{DE}} = -1 + \lambda^2/3$. For p away from 0 (like the case $p \geq 1$), the evolution of w_{DE} in the tracking freezing model explained above can be clearly distinguished from that in the Λ CDM model.

The analytic solution (10.32) of the tracker contains only two parameters $w_{(0)}$ and $\Omega_{\phi 0}$, so it is convenient to place bounds on these parameters from observations.

The observational constraints on tracking freezing models were carried out in Refs. [15, 18] by using the analytic solution (10.32). With the quintessence prior $w_{(0)} > -1$, the joint data analysis of SN Ia+CMB (WMAP)+BAO showed that the tracker equation of state is constrained to be $w_{(0)} < -0.964$ (95% CL). This bound translates to $p < 0.075$ for the inverse power-law potential (10.27), so the models with integer $p (\geq 1)$ are excluded from the data. The likelihood analysis of Ref. [15] showed that the best-fit model corresponds to the case $w_{(0)} = -1$, so the tracking freezing models are not particularly favored over the Λ CDM model. Without setting the prior $w_{(0)} > -1$, the best-fit model parameters were found to be $w_{(0)} = -1.097$ and $\Omega_{\phi 0} = 0.717$ [15]. The region $w_{(0)} < -1$ is favored by the data, but this phantom tracker equation of state cannot be realized by the quintessence field.

10.1.3.2. *Scaling freezing models*

In Sec. 10.1.2, we showed that, for the exponential potential (10.16), there exists the scaling solution along which the field density parameter Ω_ϕ stays a constant value $3(1+w_m)/\lambda^2$. This is regarded as a special case of the tracker given by Eq. (10.23) with $w_{\text{DE}} = w_m$ and constant λ . In this case, the Universe does not enter the stage of cosmic acceleration because the field equation of state is the same as that of the background fluid.

It is possible to alleviate this problem for the double exponential potential [19]

$$V(\phi) = V_1 e^{-\lambda_1 \phi/M_{\text{Pl}}} + V_2 e^{-\lambda_2 \phi/M_{\text{Pl}}}, \quad (10.33)$$

where λ_i and V_i ($i = 1, 2$) are constants (see also Refs. [20–22]). We consider the case in which the slopes λ_1 and λ_2 are in the ranges $\lambda_1 \gg 1$ and $\lambda_2 \lesssim 1$. In the early cosmological epoch, the steep exponential potential $V_1 e^{-\lambda_1 \phi/M_{\text{Pl}}}$ dominates over another exponential potential $V_2 e^{-\lambda_2 \phi/M_{\text{Pl}}}$. Then, the solution first enters the scaling regime characterized by $\Omega_\phi = 3(1+w_m)/\lambda_1^2$. We recall that this scaling solution is stable for $\lambda_1^2 > 3(1+w_m)$. During the radiation era ($w_m = 1/3$) the field density parameter is $\Omega_\phi = 4/\lambda_1^2$. There is the constraint $\Omega_\phi < 0.045$ (95% CL) from the Big Bang nucleosynthesis [23], so this translates to the bound $\lambda_1 > 9.4$. After the end of the radiation-dominated epoch, the solution enters the scaling matter era characterized by $\Omega_\phi = 3/\lambda_1^2$.

At late times, the presence of another exponential potential $V_2 e^{-\lambda_2 \phi/M_{\text{Pl}}}$ leads to the exit from the scaling matter era. For $\lambda_2^2 < 2$, the solution finally approaches another stable fixed point (c) derived in Sec. 10.1.2, so the Universe enters the stage of accelerated expansion. The onset of the transition from the scaling matter era to the epoch of cosmic acceleration depends on the parameters λ_1 , λ_2 , and the ratio V_2/V_1 . The transition redshift is not very sensitive to the choice of V_2/V_1 , so we can set $V_2 = V_1$ without losing generality. In Fig. 10.2, we plot the evolution of w_{DE} for three different values of λ_1 with $\lambda_2 = 0$. In the early matter era the field equation of state w_{DE} is close to $w_m = 0$, but there is the transition to the de Sitter

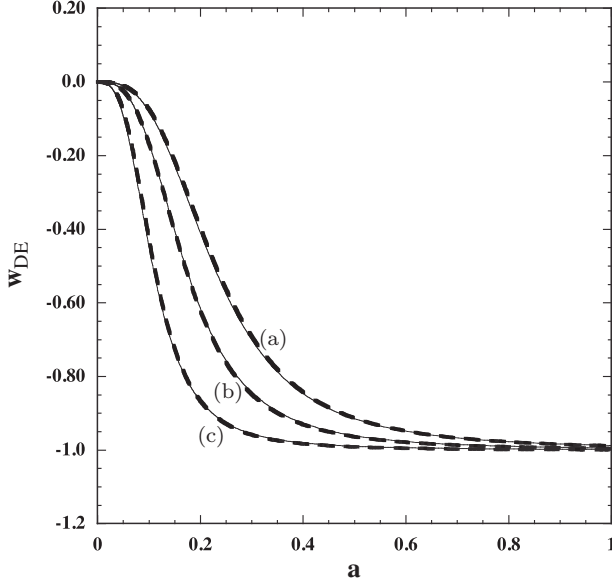


Fig. 10.2. The field equation of state w_{DE} versus a for the double exponential potential (10.33) with (a) $\lambda_1 = 10$, $\lambda_2 = 0$, (b) $\lambda_1 = 15$, $\lambda_2 = 0$, and (c) $\lambda_1 = 30$, $\lambda_2 = 0$. The solid curves are the numerically integrated solutions, whereas the dashed curves show the results derived from the parametrization (10.34) with $w_p = 0$ and $w_f = -1$. Each dashed curve corresponds to (a) $a_t = 0.23$, $\tau = 0.33$, (b) $a_t = 0.17$, $\tau = 0.33$, and (c) $a_t = 0.11$, $\tau = 0.32$.

attractor. For larger λ_1 , the transition of w_{DE} to the value -1 occurs at an earlier cosmological epoch.

It is possible to accommodate the above variation of w_{DE} with the parametrization (5.24), where τ (> 0) is the transition width, w_p and w_f are asymptotic values of w_{DE} in the past and future, respectively. The scaling solution during the matter era corresponds to $w_p = 0$. For $\lambda_2 = 0$ we have $w_f = -1$, so the dark energy equation of state describing the transition from $w_{\text{DE}} = 0$ to $w_{\text{DE}} = -1$ is given by

$$w_{\text{DE}}(a) = -1 + \left[1 + (a/a_t)^{1/\tau}\right]^{-1}. \quad (10.34)$$

As we see in Fig. 10.2, the parametrization (10.34) reproduces the numerical solutions of w_{DE} very well for suitable choices of a_t and τ [15]. For the models with $\lambda_2 = 0$ the transition width is around $\tau \approx 0.33$, while the transition scale factor a_t depends on the value of λ_1 .

Using the parametrization (10.34) with $\tau = 0.33$, the joint data analysis based on SN Ia, CMB (WMAP), and BAO data showed that the transition redshift is constrained to be $a_t < 0.23$ (95% CL) [15]. The case (a) plotted in Fig. 10.2 corresponds to the marginal case in which the model is within the 95% CL observational contour. The earlier transition like the case (c) fits the data better. In Ref. [15], the best-fit model parameters were found to be $a_t = 0$ and $\Omega_m^{(0)} = 0.27$, so it corresponds to the

Λ CDM model. For $\lambda_2 > 0$, the likelihood analysis was also performed in Ref. [15] without resorting to the parametrization (5.24), in which case the model parameters were constrained to be $\lambda_1 > 11.7$, $\lambda_2 < 0.539$, and $0.256 < \Omega_m^{(0)} < 0.279$ (95% CL). For $\lambda_2 \gtrsim 0.5$, the deviation of w_{DE} from -1 tends to be significant at late times, so such models are disfavored from the data.

10.1.3.3. Thawing models

In thawing quintessence models, the field has been nearly frozen by the Hubble friction until recently. Since $w_{\text{DE}} \simeq -1$ in this regime, this is one of the fixed points of (10.19). The representative model of this class is the potential arising from the pseudo-Nambu-Goldstone boson (PNGB) [24]:

$$V(\phi) = \mu^4 \left[1 + \cos\left(\frac{\phi}{f}\right) \right], \quad (10.35)$$

where μ and f are constants characterizing the energy scale and the mass scale of spontaneous symmetry breaking, respectively. The mass squared of the field is given by $m_\phi^2 \equiv d^2V/d\phi^2 = -(\mu^4/f^2) \cos(\phi/f)$, which is negative for $0 < \phi < (\pi/2)f$. If the field initially exists around $\phi = 0$, it follows that $m_\phi^2 \simeq -\mu^4/f^2$.

If today's acceleration of the Universe is realized by the potential (10.35) around $\phi = 0$, today's Hubble parameter H_0 is related to the mass scale μ , as $H_0^2 \simeq \mu^4/M_{\text{pl}}^2$. Then, the mass squared around $\phi = 0$ is given by

$$m_\phi^2 \simeq -\frac{M_{\text{pl}}^2}{f^2} H_0^2. \quad (10.36)$$

The slow-roll parameter η_V defined by Eq. (4.103) is smaller than the order of 1 for the realization of cosmic acceleration. For the potential (10.35), the condition $|\eta_V| \lesssim 1$ translates to $f \gtrsim M_{\text{pl}}$ around $\phi = 0$. On using Eq. (10.36), the field mass is constrained to be

$$|m_\phi| \lesssim H_0 \approx 10^{-33} \text{ eV}. \quad (10.37)$$

Since the field is very light, it has been nearly frozen during most of the cosmic expansion history. The field starts to evolve when H decreases to the order of H_0 .

In the following, we analytically derive the solution to the dark energy equation of state w_{DE} in thawing quintessence models. For a given initial value ϕ_i of the field, we expand the potential $V(\phi)$ around $\phi = \phi_i$ up to second order as

$$V(\phi) \simeq V(\phi_i) + V_{,\phi}(\phi_i)(\phi - \phi_i) + \frac{1}{2} V_{,\phi\phi}(\phi_i)(\phi - \phi_i)^2. \quad (10.38)$$

Employing the approximation $P_\phi \simeq -\rho_\phi \simeq -V(\phi_i)$ and defining a rescaled field $u \equiv (\phi - \phi_i)a^{3/2}$, Eq. (10.3) approximately reduces to

$$\ddot{u} - \omega^2 u \simeq -a^{3/2} V_{,\phi}(\phi_i), \quad \omega = \left[\frac{3}{4} \frac{V(\phi_i)}{M_{\text{pl}}^2} - V_{,\phi\phi}(\phi_i) \right]^{1/2}. \quad (10.39)$$

Since we are considering the regime in which $|m_\phi|$ is smaller than H_0 , we assume the condition $3V(\phi_i)/(4M_{\text{pl}}^2) > V_{,\phi\phi}(\phi_i)$. As long as the deviation of w_{DE} from -1 is small such that $|w_{\text{DE}} + 1| \ll 1$, the evolution of the scale factor in thawing models can be well approximated as that of the Λ CDM model. Since in this case $\dot{a}^2 = H_0^2 a^2 [\Omega_{\phi 0} + (1 - \Omega_{\phi 0})a^{-3}]$ from Eq. (10.5), the integrated solution of the scale factor is approximately given by

$$a(t) = \left(\frac{1 - \Omega_{\phi 0}}{\Omega_{\phi 0}} \right)^{1/3} \sinh^{2/3} \left(\frac{t}{t_\Lambda} \right), \quad t_\Lambda = \frac{2M_{\text{pl}}}{\sqrt{3V(\phi_i)}}. \quad (10.40)$$

Substituting Eq. (10.40) into Eq. (10.39) and integrating it with respect to t , it follows that

$$u(t) = C_1 \sinh(\omega t) + C_2 \cosh(\omega t) + \sqrt{\frac{1 - \Omega_{\phi 0}}{\Omega_{\phi 0}}} \frac{V_{,\phi}(\phi_i) t_\Lambda^2}{\omega^2 t_\Lambda^2 - 1} \sinh \left(\frac{t}{t_\Lambda} \right), \quad (10.41)$$

where C_1 and C_2 are integration constants. Equation (10.41) is valid for $\omega t_\Lambda \neq 1$, i.e., for $V_{,\phi\phi}(\phi_i) \neq 0$. Under the initial conditions $\phi(0) = \phi_i$ and $\dot{\phi}(0) = 0$, the resulting solution is given by

$$\phi(t) = \phi_i + \frac{V_{,\phi}(\phi_i)}{V_{,\phi\phi}(\phi_i)} \left[\frac{\sinh(\omega t)}{\omega t_\Lambda \sinh(t/t_\Lambda)} - 1 \right]. \quad (10.42)$$

Since $w_{\text{DE}} + 1 \simeq \dot{\phi}^2(t)/V(\phi_i)$ under the slow-roll approximation $\rho_\phi \simeq V(\phi_i)$, the field equation of state reads

$$w_{\text{DE}} \simeq -1 + \frac{3}{4} \left[\frac{V_{,\phi}(\phi_i)}{\omega t_\Lambda V_{,\phi\phi}(\phi_i)} \right]^2 \left[\frac{\omega t_\Lambda \cosh(\omega t) \sinh(t/t_\Lambda) - \sinh(\omega t) \cosh(t/t_\Lambda)}{\sinh^2(t/t_\Lambda)} \right]^2. \quad (10.43)$$

The right hand side of Eq. (10.43) can be expressed in terms of the function of a . In doing so, we introduce the dimensionless variables

$$\mathcal{A} \equiv \omega t_\Lambda = \sqrt{1 - \frac{4M_{\text{pl}}^2 V_{,\phi\phi}(\phi_i)}{3V(\phi_i)}}, \quad \mathcal{B}(a) \equiv \sqrt{1 + [(\Omega_{\phi 0})^{-1} - 1]a^{-3}}. \quad (10.44)$$

From Eq. (10.40), we obtain the relation $\omega t = \mathcal{A} \sinh^{-1} \sqrt{a^3 \Omega_{\phi 0} / (1 - \Omega_{\phi 0})}$. Then Eq. (10.43) can be expressed as [25, 26]

$$w_{\text{DE}}(a) \simeq -1 + (1 + w_0) a^{3(\mathcal{A}-1)} \mathcal{F}(a), \quad (10.45)$$

where w_0 is today's value of w_{DE} , and

$$\mathcal{F}(a) \equiv \left[\frac{(\mathcal{A} - \mathcal{B}(a))(\mathcal{B}(a) + 1)^{\mathcal{A}} + (\mathcal{A} + \mathcal{B}(a))(\mathcal{B}(a) - 1)^{\mathcal{A}}}{(\mathcal{A} - \Omega_{\phi 0}^{-1/2})(\Omega_{\phi 0}^{-1/2} + 1)^{\mathcal{A}} + (\mathcal{A} + \Omega_{\phi 0}^{-1/2})(\Omega_{\phi 0}^{-1/2} - 1)^{\mathcal{A}}} \right]^2. \quad (10.46)$$

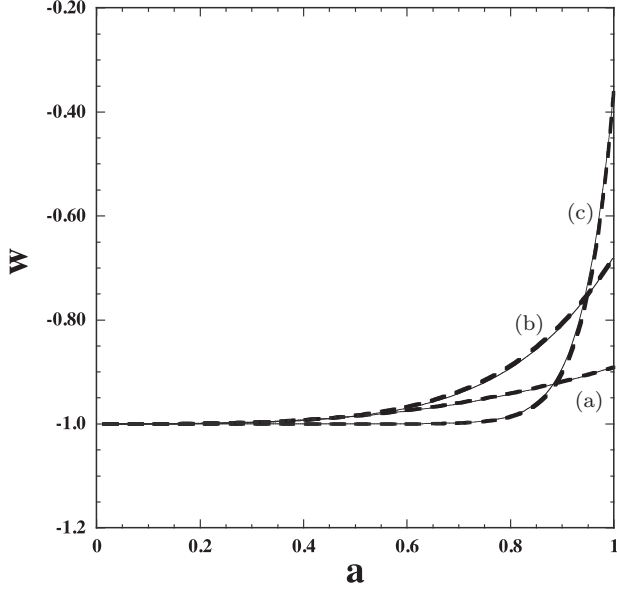


Fig. 10.3. The field equation of state w_{DE} versus a for the potential (10.35) with (a) $f/M_{\text{pl}} = 0.5$, $\phi_i/f = 0.5$ ($\mathcal{A} = 1.9$), (b) $f/M_{\text{pl}} = 0.3$, $\phi_i/f = 0.25$ ($\mathcal{A} = 2.9$), and (c) $f/M_{\text{pl}} = 0.1$, $\phi_i/f = 7.6 \times 10^{-4}$ ($\mathcal{A} = 8.2$). The solid thin lines correspond to numerically integrated solutions, whereas the bold dashed lines show results derived from the analytic solution (10.45) with $\Omega_{\phi 0} = 0.73$.

The quantity $\mathcal{A}$ contains the second derivative $V_{,\phi\phi}(\phi_i)$, so it is related to the field mass squared m_ϕ^2 . For the potential (10.35), we have $\mathcal{A} > 1$ for $0 < \phi_i/f < \pi/2$ and $\mathcal{A} < 1$ for $\pi/2 < \phi_i/f < \pi$, respectively. If $4M_{\text{pl}}^2 V_{,\phi\phi}(\phi_i)/(3V(\phi_i)) > 1$ (i.e., $\mathcal{A}^2 < 0$), it is possible to derive an analytic solution of w_{DE} similar to Eq. (10.45) by setting $\mathcal{A} = i\hat{\mathcal{A}}$ and $\hat{\mathcal{A}} = \sqrt{4M_{\text{pl}}^2 V_{,\phi\phi}(\phi_i)/(3V(\phi_i)) - 1}$ [26].

In Fig. 10.3, we show numerical solutions of w_{DE} for the potential (10.35) as well as analytic solutions derived from (10.45) for three different values of $\mathcal{A}$. Provided that $\mathcal{A} \lesssim 10$ and $w_0 \lesssim -0.3$, we find that analytic solutions can reproduce numerical solutions with high accuracy. For increasing $\mathcal{A}$ the field mass gets larger, so the variation of w_{DE} is more significant around today. For the validity of the Taylor expansion exploited for the derivation of the solution (10.45), we require the condition $|\mathcal{A} - 1| < \mathcal{O}(1)$. For the models with $V_{,\phi\phi} > 0$, analytic solutions tend to be inaccurate for smaller $\mathcal{A}$ less than 0.5.

There are three parameters w_0 , $\Omega_{\phi 0}$, and $\mathcal{A}$ in the analytic expression of Eq. (10.45). If these parameters are varied in the joint data analysis of SN Ia+CMB (WMAP)+BAO, the bound on $\mathcal{A}$ is generally weak even with the prior $0.1 < \mathcal{A} < 10$. After marginalizing over $\mathcal{A}$ without any prior on w_0 , the bounds on other two parameters were found to be $-2.18 < w_0 < -0.893$ and $0.703 < \Omega_{\phi 0} < 0.735$ (95% CL) [15]. Putting the quintessence prior $w_0 > -1$, today's dark energy equation of state was constrained to be $w_0 < -0.849$ (68% CL) and $w_0 < -0.695$ (95% CL) [15].

There has been no statistical evidence that the models with $w_0 > -1$ are favored over the Λ CDM, but the thawing models with $-1 < w_0 < -0.7$ are allowed from the data.

10.1.1.4. Particle physics models of quintessence

There were numerous attempts for the construction of particle physics models of quintessence.¹ Many of them are based on theories beyond the Standard Model of particle physics. The general requirement for the quintessence potential is that the quintessence energy density V_0 today is as small as $H_0^2 M_{\text{pl}}^2 \simeq 10^{-47} \text{ GeV}^4$. The slow-roll condition $|\eta_V| = |M_{\text{pl}}^2 V_{,\phi\phi}/V| \lesssim 1$ shows that the field mass squared $m_\phi^2 = V_{,\phi\phi}$ satisfies the condition

$$|m_\phi^2| \lesssim \frac{V_0}{M_{\text{pl}}^2} \approx H_0^2. \quad (10.47)$$

Such a ultra-light scalar field can be unstable against radiative corrections. The radiation corrections can disrupt the flatness of the potentials required for the cosmic acceleration [27, 28]. Nevertheless, as we will see below, it is not entirely hopeless to construct viable quintessence models in the framework of supersymmetric theories. In the following, we review attempts for the construction of quintessence models in supersymmetric theories.

10.1.1.4.1. Globally supersymmetric QCD theories

The inverse power-law potential (10.27) discussed in Sec. 10.1.3.1 arises in globally supersymmetric QCD theories with N_c colors and N_f ($< N_c$) flavors [29]. The matter content in this theory constitutes quarks ϕ_i ($i = 1, 2, \dots, N_f$) in fundamentals of $SU(N_c)$ and anti-quarks $\bar{\phi}_i$ in anti-fundamentals of $SU(N_c)$. The effective degrees of freedom below the gauge-symmetry breaking scale Λ are the fermion condensate fields $T_{ij} \equiv \phi_i \bar{\phi}_j$.

Our interest is the dynamics of field expectation values along perturbatively flat directions, such that $\langle \phi_{ij} \rangle = \langle \bar{\phi}_{ij}^\dagger \rangle$, where $j = 1, \dots, N_c$ is the gauge index. The supersymmetry and the anomaly-free global symmetry restricts the superpotential of the form [30]

$$W = (N_c - N_f) \left(\frac{\Lambda^{3N_c - N_f}}{\det T} \right)^{\frac{1}{N_c - N_f}}, \quad (10.48)$$

where $\det T$ is the determinant of the matrix T_{ij} . The scalar potential in globally supersymmetric theories is expressed in terms of the superpotential W as

¹This section contains some advanced topics, so readers can skip it at first reading.

Eq. (9.30), i.e.,

$$V(\phi_i, \bar{\phi}_i) = \sum_{i=1}^{N_f} (|W_{,\phi_i}|^2 + |W_{,\bar{\phi}_i}|^2). \quad (10.49)$$

Under gauge and flavor rotations, it is possible to diagonalize the field expectation values as $\langle \phi_{ij} \rangle = \langle \bar{\phi}_{ij}^\dagger \rangle = \phi_i \delta_{ij}$ for $1 \leq j \leq N_f$ and $\langle \phi_{ij} \rangle = \langle \bar{\phi}_{ij}^\dagger \rangle = 0$ for $N_f < j \leq N_c$. We take the expectation values of all N_f fields to be equal, i.e., $\langle \phi_i \rangle = \phi$ ($i = 1, \dots, N_f$), in which case $\det T = \phi^{2N_f}$. Hence the field potential (10.49) reduces to the inverse power-law potential $V(\phi) \propto \phi^{-p}$ with the index

$$p = 2 \frac{N_c + N_f}{N_c - N_f}. \quad (10.50)$$

We caution that this result is the outcome of globally supersymmetric QCD theory without including gravity. In other words, the globally supersymmetric theory should be promoted to a locally supersymmetric supergravity theory.

10.1.4.2. Quintessence in supergravity

As we explained in Sec. 9.3, the four-dimensional effective supergravity action for chiral scalar fields ϕ^i is given by Eq. (9.34). The scalar potential (9.31) depends on the Kähler potential K and the superpotential W . Since the second term in the square bracket of Eq. (9.31) is negative, this can generally be an obstacle for the realization of a positive potential required for the cosmic acceleration. However, as in no-scale models discussed in Sec. 9.3, there are cases in which the negative contribution to the potential can be cancelled by particular choices of K and W .

As the first example, we consider the Kähler potential²

$$K = -M_{\text{pl}}^2 \ln[(\varphi + \varphi^*)/M_{\text{pl}}]. \quad (10.51)$$

As we mentioned in Sec. 9.3, the Kähler potential of this form often arises for four-dimensional dilaton and axion fields in string theory. Defining $\phi = (M_{\text{pl}}/\sqrt{2}) \ln(\varphi/M_{\text{pl}})$ for the real scalar field φ , the kinetic term $\mathcal{L}_{\text{kin}} = K_{ij} \partial_\mu \varphi^i \partial^\mu \varphi^{j*}$ in the supergravity action (9.34) reduces to $\mathcal{L}_{\text{kin}} = -\partial^\mu \phi \partial_\mu \phi/2$. As in the fermion condensate model discussed in Sec. 10.1.4.1, we consider the superpotential of the form $W = \Lambda^{3+\alpha} \varphi^{-\alpha}$, where α is a constant. Then, the scalar potential (9.31) reduces to [32]

$$V(\phi) = V_0 e^{-\lambda \phi/M_{\text{pl}}}, \quad (10.52)$$

²For the Kähler potential of the form $K = \varphi \varphi^*$, it is difficult to eliminate the negative term $-3|W|^2/M_{\text{pl}}^2$ unless the specific condition $\langle W \rangle = 0$ is imposed [31].

where

$$\lambda \equiv \sqrt{2}\beta, \quad \beta \equiv 2\alpha + 1, \quad V_0 \equiv M_{\text{pl}}^{-\beta-1} \Lambda^{\beta+5} (\beta^2 - 3)/2. \quad (10.53)$$

The positivity of the potential ($V_0 > 0$) requires that $\beta > \sqrt{3}$, i.e., $\lambda > \sqrt{6}$. This requirement is incompatible with the condition $\lambda < \sqrt{2}$ for the cosmic acceleration driven by the exponential potential. For $\lambda > \sqrt{6}$, there is a scaling solution along which the field density parameter $\Omega_\phi = 3(1 + w_m)/\lambda^2$ is constant during the radiation and matter eras, but the form of the potential needs to be modified at late times to for realizing the cosmic acceleration.

To overcome this problem, Copeland *et al.* [32] considered more general Kähler potentials of the form

$$K = M_{\text{pl}}^2 [\ln(\varphi + \varphi^*)/M_{\text{pl}}]^\gamma, \quad (10.54)$$

where γ is a constant larger than 1. For simplicity, let us focus on the case $\gamma = 2$ with the superpotential $W = \Lambda^{3+\alpha} \varphi^{-\alpha}$ of a real scalar field. The kinetic term in the action (9.34) can be made canonical by defining the rescaled field $\phi \equiv \int \sqrt{2K_{\varphi\varphi^*}} d\varphi = -(2M_{\text{pl}}/3) [1 - \ln(2\varphi/M_{\text{pl}})]^{3/2}$. The field potential reduces to

$$V = \frac{M^4}{Y} [2Y^2 + (4\alpha - 7)Y + 2(\alpha - 1)^2] \exp[(1 - Y)^2 - 2\alpha(1 - Y)], \quad (10.55)$$

where $M^4 \equiv 2^{2\alpha} M_{\text{pl}}^{-2-2\alpha} \Lambda^{6+2\alpha}$ and

$$Y \equiv 1 - \ln\left(\frac{2\varphi}{M_{\text{pl}}}\right) = \left(-\frac{3\phi}{2M_{\text{pl}}}\right)^{2/3}. \quad (10.56)$$

The field is in the range $\phi < 0$. In the two regimes $|\phi| \ll M_{\text{pl}}$ and $|\phi| \gg M_{\text{pl}}$, the potential behaves as $V \propto (-\phi)^{-2/3}$ and $V \propto (-\phi)^{2/3} e^{(\phi/M_{\text{pl}})^{4/3}}$, respectively. There is a potential minimum with a positive energy density in the intermediate region. If the field is initially in the region $|\phi| \ll M_{\text{pl}}$, the scalar field enters a tracking regime driven by the power-law potential $V(\phi) \propto (-\phi)^{-2/3}$. For the initial conditions with $|\phi| \gg M_{\text{pl}}$, the presence of the exponential term $e^{(\phi/M_{\text{pl}})^{4/3}}$ multiplied by $(-\phi)^{2/3}$ leads to the scaling-like behavior [32]. In both cases the Universe finally enters the epoch of cosmic acceleration as the field approaches the potential minimum.

In supersymmetric theories, there exists a supersymmetric fermionic partner of the graviton called the gravitino [33]. The breaking of supersymmetry is related to the gravitino mass $m_{3/2}$. In the so-called gravity-mediated scenario, the supersymmetry breaking should occur at the energy scale $\sqrt{\langle F \rangle} \sim \sqrt{m_{3/2} M_{\text{pl}}} \gtrsim 10^{10}$ GeV to lift the masses of supersymmetric scalar particles above 10^2 GeV, where the F term is defined by $F^2 \equiv e^{K/M_{\text{pl}}^2} D_i W (K^{ij*}) (D_j W)^*$. To have a negligibly small vacuum energy in Eq. (9.31), the superpotential should take the form $W \sim \langle F \rangle M_{\text{pl}} \sim m_{3/2} M_{\text{pl}}^2$. Then, the superpotential $W = \Lambda^{3+\alpha} \varphi^{-\alpha}$ used above gets corrected by the term $m_{3/2} M_{\text{pl}}^2$. This gives rise to the correction of the order of $m_{3/2}^2 M_{\text{pl}}^2$ to the

scalar potential (9.31). Hence the flatness of the potential required for the late-time cosmic acceleration is disrupted.

It is possible to overcome this problem in some of the extended version of supergravity models [34–36]. In this extended scenario, the mass squared of light scalar fields can be quantized in unit of the squared of the Hubble constant H_0 of a de Sitter solution. The de Sitter solution corresponds to the extremum of an effective potential $V(\phi)$ of a scalar field ϕ . Around the extremum with the field value $\phi = 0$, the scalar potential is given by $V(\phi) = \Lambda + (1/2)m_\phi^2\phi^2$ with $\Lambda > 0$. In extended supergravity theories, there is the relation $m_\phi^2 = n\Lambda/(3M_{\text{pl}}^2)$ between the constant Λ and the field mass m_ϕ , where n is an integer. Since $H_0^2 = \Lambda/(3M_{\text{pl}}^2)$ for de Sitter solutions, the mass squared reads $m_\phi^2 = nH_0^2$. Then the scalar potential yields

$$V(\phi) = 3H_0^2 M_{\text{pl}}^2 \left(1 + \frac{n}{6} \frac{\phi^2}{M_{\text{pl}}^2} \right). \quad (10.57)$$

The integer n can be either positive or negative depending on the kind of supergravity theories [35, 36]. The constant $\Lambda = 3H_0^2 M_{\text{pl}}^2$ determines the energy scale of supersymmetry breaking. If the potential (10.57) drives today's cosmic acceleration, the supersymmetry breaking scale is as small as $\Lambda \approx 10^{-47} \text{ GeV}^4$. Then, the ultra-light mass of the order of $m_\phi = \sqrt{n}H_0 \approx 10^{-33} \text{ eV}$ can be protected against quantum corrections. The potential (10.57) belongs to a class of thawing quintessence models in which the dark energy equation of state w_{DE} starts to deviate from -1 only recently.

10.1.4.3. *Supersymmetric axion quintessence*

The light mass of quintessence can be also protected for the PNGB potential (10.35) by the $U(1)$ symmetry. The axion field can be the candidate for such a ultra-light PNGB [37–40]. When a global $U(1)$ symmetry is spontaneously broken, the axion appears as an angular massless field ϕ with an expectation value $\langle \varphi \rangle = f_s e^{i\phi/f_s}$ of a complex scalar at a scale f_s . Originally, Peccei and Quinn (PQ) [41] introduced the axion to overcome the strong CP problem in QCD [41]. The energy scale associated with the breaking of $U(1)$ symmetry of the QCD axion is much higher than the dark energy scale. In string theory many light axions are present, possibly populating each decade of mass down to the scale $H_0 \approx 10^{-33} \text{ eV}$ [40].

The energy scale μ of the potential (10.35) is as small as $\mu \simeq \sqrt{H_0 M_{\text{pl}}} \simeq 10^{-3} \text{ eV}$ for the axion potential relevant to dark energy. In the limit that $\mu \rightarrow 0$, the symmetry of the potential (10.35) becomes exact. The radiative correction, which is proportional to μ^4 , does not give rise to an explicit symmetry breaking term. Then, the small mass term $|m_\phi| \simeq \mu^2/f \lesssim 10^{-33} \text{ eV}$ relevant to dark energy can be protected against the radiative correction.

In supersymmetric theories, there were several attempts for explaining the small mass scale μ of the order of 10^{-3} eV [37–39, 42]. From the two fundamental

scales $M_{\text{pl}} \approx 10^{18}$ GeV (Planck scale) and $v \approx 10^3$ GeV (electroweak scale), we can think of the induced seesaw scale $v^2/M_{\text{pl}} \approx 10^{-3}$ eV. This is of the same order as $\mu \approx 10^{-3}$ GeV. Assuming the relation $\mu \approx v^2/M_{\text{pl}}$ and $f \approx M_{\text{pl}}$, it follows that $|m_\phi^2| \approx \mu^4/f^2 \approx v^8/M_{\text{pl}}^6$. Then the field mass can be estimated as $|m_\phi| \approx v^4/M_{\text{pl}}^3 \approx 10^{-33}$ eV, which is of the same order as the quintessence mass.

To justify the relation $\mu \approx v^2/M_{\text{pl}}$, Hall *et al.* [42] proposed a supersymmetric model with the axion in a hidden sector. If the supersymmetry breaking in Nature occurs around the TeV scale $v \approx 10^3$ GeV, then any sector of the theory feeling this symmetry breaking indirectly through gravity mediation has the effective supersymmetry breaking scale $m_B = v^2/M_{\text{pl}}$. In the presence of a hidden sector with a supersymmetric gauge interaction acting on chiral superfields, the squarks and gluinos receive masses of the order of m_B after the supersymmetry breaking. It is also natural to assume that the quark acquires the same order of mass.

If the $U(1)$ symmetry in the hidden sector is broken with the breaking scale f of the order of M_{pl} , the interacting Lagrangian between the axion ϕ and the quarks q, q^c at the scale Λ is given by

$$\mathcal{L}_{\text{axion}} = m_q qq^c e^{i\phi/f} + \text{h.c.}, \quad (10.58)$$

where m_q is the quark mass of the order of m_B , and “h.c.” means the hermitian conjugate. The axion has a $U(1)$ symmetry $U(1)_{\text{PQ}}$ broken around $f \approx M_{\text{pl}}$, while the quark bilinear qq^c carries the axial $U(1)$ symmetry $U(1)_A$. The interaction (10.58) leads to the breaking of $U(1)_{\text{PQ}} \times U(1)_A$ symmetry explicitly. Assuming that the mass of at least one quark flavor in Eq. (10.58) is smaller than Λ , a quark condensate with $\langle qq^c \rangle \approx \Lambda^3 e^{i\phi'/\Lambda}$ is formed with an angular field ϕ' . Then the interaction (10.58) gives rise to the potential

$$V = \mu^4 \cos\left(\frac{\phi}{f} + \frac{\phi'}{\Lambda}\right), \quad (10.59)$$

where $\mu^4 = m_q \Lambda^3$ and $\Lambda \approx m_B$. Then, the scale μ is of the order of $\mu \approx m_B = v^2/M_{\text{pl}} \approx 10^{-3}$ eV, as required for quintessence.

We have thus shown that the thawing models described by the potentials (10.35) and (10.57) can be good theoretical candidates for quintessence with controlled radiative corrections. As we discussed in Sec. 10.1.3.3, the thawing models with today’s dark energy equation of state smaller than -0.7 are also compatible with the joint data analysis of SN Ia+CMB+BAO. The current observational data are not yet sufficiently accurate to distinguish between the thawing quintessence and the Λ CDM model, but this situation will be improved in future observations.

10.2. k-essence

In quintessence, the acceleration of the Universe is realized by the potential energy of a canonical scalar field. It is also possible to drive the cosmic acceleration with a

non-canonical kinetic term of a scalar field ϕ — which is dubbed k-essence [43–45]. The general theories of k-essence in the presence of matter fields Ψ_m (with the action S_m) are expressed as

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} R + P(\phi, X) \right] + S_m(g_{\mu\nu}, \Psi_m), \quad (10.60)$$

where $P(\phi, X)$ is a function with respect to ϕ and

$$X = -\frac{1}{2} g^{\mu\nu} \nabla_\mu \phi \nabla_\nu \phi. \quad (10.61)$$

As we derived in Eq. (6.56), the energy density and the pressure of k-essence on the FLRW background are given, respectively, by

$$\rho_\phi = 2XP_{,X} - P, \quad P_\phi = P. \quad (10.62)$$

Then, the field equation of state reads

$$w_{\text{DE}} = \frac{P}{2XP_{,X} - P}. \quad (10.63)$$

If the condition $|2XP_{,X}| \ll |P|$ is satisfied, w_{DE} is close to -1 . The quintessence corresponds to the Lagrangian density $P = X - V(\phi)$, in which case the cosmic acceleration with $w_{\text{DE}} \simeq -1$ can be realized for $2X \ll |P| \approx V$. For k-essence the kinetic term X is not necessarily small, but as long as $P_{,X}$ is close to 0, it is possible to realize w_{DE} close to -1 .

We assume that the scalar field ϕ is minimally coupled to matter. As a matter action S_m , we take into account a perfect fluid whose background energy density and pressure are given, respectively, by ρ_m and P_m . Then, the Einstein equations on the flat FLRW spacetime yield

$$3M_{\text{pl}}^2 H^2 = 2XP_{,X} - P + \rho_m, \quad (10.64)$$

$$2M_{\text{pl}}^2 \dot{H} = -(2XP_{,X} + \rho_m + P_m), \quad (10.65)$$

The continuity equations of the field ϕ and the perfect fluid are given, respectively, by

$$\dot{\rho}_\phi + 3H(\rho_\phi + P_\phi) = 0, \quad (10.66)$$

$$\dot{\rho}_m + 3H(\rho_m + P_m) = 0, \quad (10.67)$$

Among Eqs. (10.64)–(10.67), three of them are independent.

As an example of k-essence, let us consider the ghost condensate model [46] given by

$$P = -X + \frac{X^2}{M^4}, \quad (10.68)$$

where M is a constant having a dimension of mass. In this model there is the negative kinetic term $-X$, but the existence of the term X^2/M^4 can avoid the appearance of ghosts (which will be discussed in Sec. 10.2.1). Since $P_{,X} = -1 + 2X/M^4$, there exists a de Sitter point ($w_{\text{DE}} = -1$) characterized by $X = M^4/2$. At this point the field energy density is given by $\rho_\phi = M^4/4$ with the pressure $P_\phi = -M^4/4$, so the present cosmic acceleration occurs for $M \approx 10^{-3}$ eV.

The ghost condensate (10.68) is a purely kinetic-driven inflationary scenario in which the acceleration of the Universe is driven by the field kinetic energy. There are models in which the Lagrangian density contains the ϕ dependence as well as X . Two representative models of the latter class are given by

$$(i) \quad P = -V(\phi)\sqrt{-\det(g_{\mu\nu} + \nabla_\mu\phi\nabla_\nu\phi)}, \quad (10.69)$$

$$(ii) \quad P = -f(\phi)^{-1}\sqrt{1 - 2f(\phi)\dot{X}} + f(\phi)^{-1} - V(\phi), \quad (10.70)$$

where $V(\phi)$ and $f(\phi)$ are functions of ϕ . The scalar field ϕ in the model (i), which is called a tachyon, arises in open string theory living on a non-BPS D3-brane [47–49]. The model (ii) is called the Dirac-Born-Infeld (DBI) scenario in which the movement of a probe D3-brane in the radial direction of the AdS_5 spacetime is described by the action (10.70) [50, 51]. In both cases, the existence of the potential $V(\phi)$ is important to drive the acceleration of the Universe. For the functions $V(\phi)$ and $f(\phi)$ arising in the original setup of string theory, the models (i) and (ii) are not able to account for the late-time cosmic acceleration. Allowing the freedom to modify the functions $V(\phi)$ and $f(\phi)$, it is possible for such models to be responsible for dark energy [52–58].

10.2.1. Conditions for avoiding ghosts and instabilities

In this section, we derive theoretically consistent conditions for k-essence on the flat FLRW background. In doing so, we consider the perturbation $\delta\phi$ of the field ϕ and scalar metric perturbations with the line element (6.13). We choose the unitary gauge $\delta\phi = 0$ to fix the temporal component of the gauge-transformation vector ξ^μ . The gauge $E = 0$ is chosen to fix the spatial component of ξ^μ , in which case the perturbed metric is given by Eq. (6.143) with three scalar metric perturbations A , B , and $\mathcal{R}$. We expand the action (10.60) up to second order in perturbations without the matter action S_m , so that $\rho_m = 0$ and $P_m = 0$ in the background Eqs. (10.64)–(10.67). The second-order action of k-essence reads

$$\begin{aligned} S^{(2)} = & \int d\eta d^3x a^2 [-3M_{\text{pl}}^2 \mathcal{R}'^2 + 2M_{\text{pl}}^2 \mathcal{R}' \partial^2 B - 2M_{\text{pl}}^2 \mathcal{H} A \partial^2 B + M_{\text{pl}}^2 (\partial \mathcal{R})^2 \\ & - 2M_{\text{pl}}^2 A \partial^2 \mathcal{R} + 6M_{\text{pl}}^2 \mathcal{H} A \mathcal{R}' + \{a^2 X (P_{,X} + 2X P_{,XX}) - 3M_{\text{pl}}^2 \mathcal{H}^2\} A^2], \end{aligned} \quad (10.71)$$

where $\mathcal{H} = aH$, and a prime represents a derivative with respect to $\eta = \int a^{-1} dt$. The last term of Eq. (10.71) was modified compared to Eq. (6.144) derived for quintessence. Varying the action (10.71) with respect to B , we obtain

$$A = \frac{\mathcal{R}'}{\mathcal{H}}. \quad (10.72)$$

Substituting Eq. (10.72) into Eq. (10.71) and using the background equation $M_{\text{pl}}^2(\mathcal{H}' - \mathcal{H}^2) = -a^2 X P_{,X}$, the action (10.71) reduces to the simple form (up to boundary terms):

$$S^{(2)} = \int d\eta d^3x a^2 Q_s [\mathcal{R}'^2 - c_s^2 (\partial \mathcal{R})^2], \quad (10.73)$$

where

$$Q_s \equiv \frac{a^2}{\mathcal{H}^2} X(P_{,X} + 2X P_{,XX}), \quad c_s^2 \equiv \frac{P_{,X}}{P_{,X} + 2X P_{,XX}}. \quad (10.74)$$

The condition for avoiding the scalar ghost is $Q_s > 0$, i.e.,

$$P_{,X} + 2X P_{,XX} > 0. \quad (10.75)$$

The Laplacian instability for small-scale perturbations is absent for $c_s^2 > 0$. Under the no-ghost condition (10.75), the condition $c_s^2 > 0$ translates to

$$P_{,X} > 0. \quad (10.76)$$

We require the two conditions (10.75) and (10.76) for theoretical consistency of k-essence. If they are violated, the vacuum is unstable under a catastrophic production of ghosts and photon pairs [10, 11]. Under the condition (10.76) with the negative pressure P , it follows from Eq. (10.63) that the field equation of state is in the range

$$w_{\text{DE}} > -1, \quad (10.77)$$

so that the phantom equation of state ($w_{\text{DE}} < -1$) is not realized.

The quintessence corresponds to the Lagrangian density $P = X - V(\phi)$, so the two conditions (10.75) and (10.76) are automatically satisfied. For the ghost scalar field characterized by $P = -X - V(\phi)$, neither (10.75) nor (10.76) is satisfied. As we already mentioned, the existence of higher-order terms in X besides $-X$ can alleviate this problem.

Let us consider the diatonic ghost condensate model given by the Lagrangian density [59]

$$P = -X + e^{\lambda\phi/M_{\text{pl}}} \frac{X^2}{M^4}, \quad (10.78)$$

where λ and M are constants. In the limit that $\lambda \rightarrow 0$, the ghost condensate model (10.68) is recovered. The action of low-energy effective string theory contains higher-order derivative terms like $(\nabla_\mu \phi \nabla^\mu \phi)^2$ arising from α' and loop corrections to the tree-level string action [60]. A dilaton field ϕ , which controls the strength of string

coupling, is coupled to the Ricci scalar R of the form $e^{\lambda\phi/M_{\text{Pl}}} R$. This string frame action can be transformed to the action in the Einstein frame in which the dilaton does not have a direct coupling to gravity (see Sec. 11.2.1 for the conformal transformation). The Lagrangian density of the form (10.78) can arise after transforming the low-energy effective string action to that in the Einstein frame [43, 59].

For the model (10.78), we have $P_{,X} + 2XP_{,XX} = -1 + 6e^{\lambda\phi/M_{\text{Pl}}} X/M^4$ and $P_{,X} = -1 + 2e^{\lambda\phi/M_{\text{Pl}}} X/M^4$, so the conditions (10.75) and (10.76) are satisfied for

$$e^{\lambda\phi/M_{\text{Pl}}} \frac{X}{M^4} \geq \frac{1}{2}. \quad (10.79)$$

Since the field energy density is given by $\rho_\phi = -X + 3e^{\lambda\phi/M_{\text{Pl}}} X^2/M^4$, the field equation of state reads

$$w_{\text{DE}} = \frac{1 - e^{\lambda\phi/M_{\text{Pl}}} X/M^4}{1 - 3e^{\lambda\phi/M_{\text{Pl}}} X/M^4}, \quad (10.80)$$

which is in the range $-1 \leq w_{\text{DE}} < 1/3$ under the condition (10.79). Hence the phantom equation of state ($w_{\text{DE}} < -1$) is not realized under theoretical consistent conditions. The condition for the cosmic acceleration ($-1 \leq w_{\text{DE}} < -1/3$) translates to $1/2 \leq e^{\lambda\phi/M_{\text{Pl}}} X/M^4 < 2/3$.

In Sec. 10.1, we showed that the thawing quintessence models are allowed from the observational data, whereas the freezing quintessence models with w_{DE} away from -1 are disfavored. As we will see in Sec. 10.2.2, the diatonic ghost condensate model (10.78) belongs to a class of thawing k-essence models.

10.2.2. Cosmological dynamics of dilatonic ghost condensate

As an example of k-essence, we study the cosmological dynamics of diatonic ghost condensate given by the Lagrangian (10.78) [59]. For the matter action, we take into account radiation (energy density ρ_r and pressure $\rho_r/3$) and non-relativistic matter (energy density ρ_m and pressure 0). In the background equations (10.64)–(10.67), we just need to replace $\rho_m \rightarrow \rho_m + \rho_r$ and $P_m \rightarrow \rho_r/3$. We introduce the following dimensionless variables

$$x_1 \equiv \frac{\dot{\phi}}{\sqrt{6}H M_{\text{Pl}}}, \quad x_2 \equiv \frac{\dot{\phi}^2 e^{\lambda\phi/M_{\text{Pl}}}}{2M^4}. \quad (10.81)$$

The Friedmann equation (10.64) can be written in the form $\Omega_\phi + \Omega_m + \Omega_r = 1$, where

$$\Omega_\phi \equiv \frac{\rho_\phi}{3M_{\text{Pl}}^2 H^2} = x_1^2 (-1 + 3x_2), \quad (10.82)$$

and $\Omega_m \equiv \rho_m/(3M_{\text{Pl}}^2 H^2)$, $\Omega_r \equiv \rho_r/(3M_{\text{Pl}}^2 H^2)$. From Eqs. (10.65) and (10.80), the effective equation of state $w_{\text{eff}} = -1 - 2\dot{H}/(3H^2)$ and the field equation of state are

given, respectively, by

$$w_{\text{eff}} = -x_1^2(1 - x_2) + \frac{1}{3}\Omega_r, \quad w_{\text{DE}} = \frac{1 - x_2}{1 - 3x_2}. \quad (10.83)$$

The dynamical variables x_1, x_2, Ω_r obey the differential equations

$$\frac{dx_1}{d\mathcal{N}} = x_1 \frac{3(1 + 2x_2 - \sqrt{6}\lambda x_1 x_2) + [3x_1^2(x_2 - 1) + \Omega_r](6x_2 - 1)}{2(6x_2 - 1)}, \quad (10.84)$$

$$\frac{dx_2}{d\mathcal{N}} = x_2 \frac{6(1 - 2x_2) - \sqrt{6}\lambda x_1(1 - 3x_2)}{6x_2 - 1}, \quad (10.85)$$

$$\frac{d\Omega_r}{d\mathcal{N}} = \Omega_r[\Omega_r - 1 + 3x_1^2(x_2 - 1)], \quad (10.86)$$

where $\mathcal{N} = \ln a$. The ghost and the Laplacian instability are absent under the condition (10.79), i.e., $x_2 \geq 1/2$.

From Eqs. (10.84) and (10.85), there are two fixed points $(x_1, x_2) = (0, 0)$ and $(x_1, x_2) = (0, 1/2)$, both of which obey $\Omega_\phi = 0$. The former does not satisfy the condition $x_2 \geq 1/2$, so we focus on the latter one. From Eq. (10.86), the fixed points corresponding to the radiation and matter eras are given, respectively, by

$$(a) \ (x_1, x_2, \Omega_r) = (0, 1/2, 1), \quad w_{\text{eff}} = 1/3, \quad (10.87)$$

$$(b) \ (x_1, x_2, \Omega_r) = (0, 1/2, 0), \quad w_{\text{eff}} = 0. \quad (10.88)$$

At these points, the dark energy equation of state w_{DE} is equivalent to -1 from Eq. (10.83). Even if the field does not have the scalar potential, it is possible to realize $w_{\text{DE}} = -1$ due to the existence of a non-canonical kinetic term. In the early Universe we have $x_1 \ll 1$, but with the decrease of the Hubble parameter, the quantity x_1 increases to drive the late-time cosmic acceleration.

The fixed point relevant to the cosmic acceleration satisfying the theoretically consistent condition $x_2 \geq 1/2$ is given by

$$(c) \ (x_1, x_2, \Omega_r) = \left(-\frac{\sqrt{6}}{4}\lambda f_-(\lambda), \frac{1}{2} + \frac{1}{16}\lambda^2 f_+(\lambda), 0 \right), \quad (10.89)$$

where

$$f_\pm(\lambda) \equiv 1 \pm \sqrt{1 + \frac{16}{3\lambda^2}}. \quad (10.90)$$

At this point, we have

$$w_{\text{eff}} = w_{\text{DE}} = -\frac{8 - \lambda^2 f_+(\lambda)}{8 + 3\lambda^2 f_+(\lambda)}, \quad \Omega_\phi = 1, \quad \Omega_m = 0. \quad (10.91)$$

The cosmic acceleration occurs for $-1 \leq w_{\text{eff}} < -1/3$, which translates to the condition $0 \leq \lambda < \sqrt{6}/3$. The fixed point (c) is stable for $0 \leq \lambda < \sqrt{3}$. This means

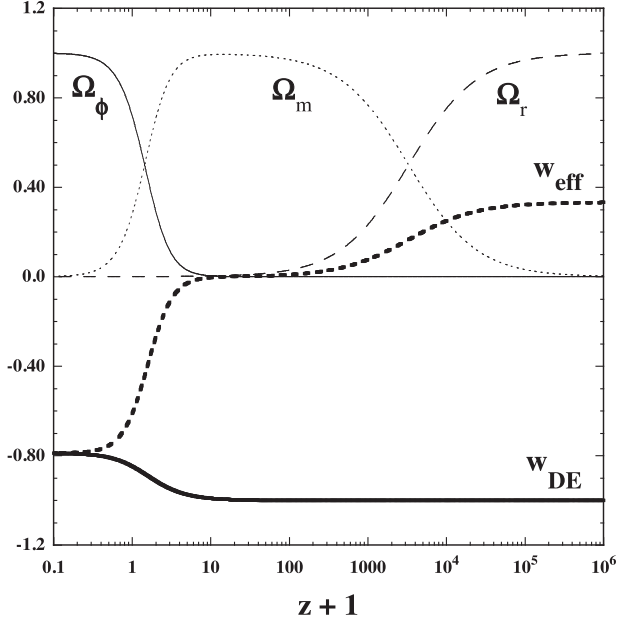


Fig. 10.4. Evolution of w_{eff} , w_{DE} , Ω_ϕ , Ω_m , Ω_r versus $z+1$ for the dilatonic ghost condensate model (10.78) with $\lambda = 0.2$. The initial conditions are chosen to be $x_1 = 6 \times 10^{-11}$, $x_2 = 0.5 + 1 \times 10^{-9}$, and $\Omega_r = 0.999$ at the redshift $z = 1.65 \times 10^6$.

that, as long as the point (c) satisfies the condition for the cosmic acceleration, it is a stable attractor.

Besides the points (a), (b) and (c), there is another fixed point $(x_1, x_2, \Omega_r) = (\sqrt{6}/(2\lambda), 1, 0)$ with $\Omega_\phi = 3/\lambda^2$, $\Omega_m = 1 - 3\lambda^2$, and $w_{\text{DE}} = 0$. This is a scaling matter solution along which the ratio Ω_ϕ/Ω_m is a non-zero constant. Existence of the scaling solution requires the condition $\lambda > \sqrt{3}$, but in this case the solution does not exit from the scaling era to approach the fixed point (c) with the cosmic acceleration.

The above discussion shows that the Universe evolves according to the sequence of the fixed points (a) $\rightarrow$ (b) $\rightarrow$ (c). In fact, this can be confirmed in Fig. 10.4 in which the evolution of w_{eff} , w_{DE} , Ω_ϕ , Ω_m , Ω_r is plotted for $\lambda = 0.2$ with the initial value of x_2 close to $+1/2$. The dilatonic ghost condensate belongs to a class of thawing k-essence models in which w_{DE} is initially close to -1 and it starts to deviate from -1 at late times. The k-essence energy density dominates over the background matter density after the quantity x_1 grows to the order of unity.

For $\lambda = 0.2$, the analytic estimation (10.91) shows that $w_{\text{DE}} = w_{\text{eff}} = -0.788$ at the fixed point (c). This is in good agreement with the numerical result plotted in Fig. 10.4. In the limit that $\lambda \rightarrow 0$, the dilatonic ghost condensate model recovers the Λ CDM model. For larger λ , the deviation of w_{DE} from -1 at the point (c) tends to be larger. Since the evolution of w_{DE} is similar to that in thawing quintessence models

discussed in Sec. 10.1.3.3, today's dark energy equation of state is observationally constrained to be $w_{\text{DE}}(z=0) \lesssim -0.7$. On using the criterion $w_{\text{DE}} < -0.7$ at the point (c), the parameter λ is constrained to be $\lambda < 0.3$.

10.2.3. *Purely kinetic k-essence*

In this section, we consider a purely kinetic k-essence scenario in which the Lagrangian P is a function of X alone, i.e.,

$$P = P(X). \quad (10.92)$$

On using the fact that the field energy density is given by $\rho = 2XP_{,X} - P$, the adiabatic sound speed squared $c_a^2 = \dot{P}/\dot{\rho}$ reads

$$c_a^2 = \frac{P_{,X}}{P_{,X} + 2XP_{,XX}}. \quad (10.93)$$

From Eqs. (6.57) and (6.59), the linear perturbations of ρ and P are given, respectively, by $\delta\rho = (P_{,X} + 2XP_{,XX})\delta X$ and $\delta P = P_{,X}\delta X$ for the Lagrangian (10.92), so the sound speed squared $c_s^2 = \delta P/\delta\rho$ is equivalent to the adiabatic sound speed squared (10.93). In this case there is no entropy perturbation as discussed in Sec. 6.6, so the purely kinetic k-essence with the Lagrangian (10.92) behaves as a perfect fluid for the linear perturbation on the FLRW background.

For example, let us first consider the Lagrangian density [61]

$$P(X) = b_1 X^2, \quad (10.94)$$

where b_1 is a constant. In this case, the field equation of state $w_\phi = P/(2XP_{,X} - P)$ and the sound speed squared c_s^2 are given, respectively, by

$$w_\phi = \frac{1}{3}, \quad c_s^2 = \frac{1}{3}. \quad (10.95)$$

Hence the scalar field with the Lagrangian (10.94) behaves as a perfect fluid of radiation. The two conditions (10.75) and (10.76) are satisfied for $b_1 > 0$.

The next example is the Lagrangian density [62]

$$P(X) = b_2 (X - X_0)^2, \quad (10.96)$$

where b_2 and X_0 (> 0) are constants. In this case we have

$$w_\phi = \frac{X - X_0}{3X + X_0}, \quad c_s^2 = \frac{X - X_0}{3X - X_0}, \quad (10.97)$$

with the field energy density $\rho = b_2(X - X_0)(3X + X_0)$. As long as X is close to X_0 , the scalar field behaves as a non-relativistic matter with $w_\phi \simeq 0$ and $c_s^2 \simeq 0$. The conditions (10.75) and (10.76) translate to $b_2(X - X_0) > 0$ and $b_2(3X - X_0) > 0$, respectively, which are satisfied for $b_2 > 0$ and $X > X_0$. The model described by the Lagrangian (10.96) works as perfect-fluid dark matter.

Let us consider another model in which a constant term $-b_0$ is present to the Lagrangian (10.96) [62]:

$$P(X) = -b_0 + b_2 (X - X_0)^2, \quad (10.98)$$

where $X_0 > 0$. As in the model (10.96), the conditions (10.75) and (10.76) are satisfied for $b_2 > 0$ and $X > X_0$. We are considering the regime in which X is around X_0 , i.e.,

$$X = X_0[1 + \epsilon(t)], \quad (10.99)$$

where $0 < \epsilon(t) \ll 1$. For the purely kinetic k-essence Lagrangian density (10.92), the field equation (10.66) reduces to

$$(P_{,X} + 2XP_{,XX})\dot{X} + 6HXP_{,X} = 0. \quad (10.100)$$

For the Lagrangian (10.98), we substitute Eq. (10.99) into Eq. (10.100) and pick up terms linear in ϵ . Then, the variable ϵ satisfies the differential equation $\dot{\epsilon} = -3H\epsilon$. The solution to this equation is given by

$$\epsilon(t) = \epsilon_1 \left(\frac{a_1}{a} \right)^3, \quad (10.101)$$

where ϵ_1 and a_1 are positive constants. This means that X approaches X_0 with time, so the pressure approaches the constant $-b_0$. Provided that $b_0 > 0$, the constant term $-b_0$ works as a cosmological constant responsible for the late-time cosmic acceleration. For the solution (10.101), the field energy density is approximately given by $\rho \simeq b_0 + 4b_2X_0^2\epsilon_1(a_1/a)^3$. Then, at linear order in ϵ , the field equation of state $w_\phi = P/\rho$ reduces to

$$w_\phi \simeq - \left[1 + \frac{4b_2}{b_0} X_0^2 \epsilon_1 \left(\frac{a_1}{a} \right)^3 \right]^{-1}. \quad (10.102)$$

In the early matter era, w_ϕ is close to 0, so the k-essence field behaves as dark matter. Since w_ϕ approaches -1 at late times, the same field behaves as dark energy. The late-time cosmic acceleration is realized by adding the cosmological constant term $-b_0$ to the Lagrangian (10.96), but the unified description of dark matter and dark energy in terms of a single field ϕ is of some interest.

The purely kinetic k-essence (10.92) is equivalent to the perfect fluid at linear order in cosmological perturbations. To study the evolution of the matter density contrast $\delta = \delta\rho/\rho$, we can resort to the discussion of gravitational clusterings given in Sec. 8.2. For the perturbations deep inside the Hubble radius ($k \gg aH$), the perturbation δ obeys the differential equation (8.22), i.e.,

$$\ddot{\delta} + 2H\dot{\delta} + \left(c_s^2 \frac{k^2}{a^2} - 4\pi G\rho \right) \delta = 0. \quad (10.103)$$

The sound speed squared for the model (10.98) is the same as that of the model (10.96) and hence

$$c_s^2 \simeq \frac{\epsilon(t)}{2} = \frac{\epsilon_1}{2} \left(\frac{a_1}{a} \right)^3. \quad (10.104)$$

Since we used the condition $\epsilon(t) \ll 1$ for the derivation of the above solutions, c_s^2 is much smaller than 1. Since $\epsilon(t)$ is in proportion to a^{-3} , c_s^2 decreases toward 0. Since the Jeans length defined by Eq. (8.23) becomes sufficiently small, the density contrast δ grows by the gravitational instability for most of the modes relevant to the observed large-scale structures. As long as $\epsilon(t) \ll 1$, the structure formation occurs in a similar way to that driven by the CDM with a negligible pressure.

The purely kinetic k-essence model (10.98) corresponds to a unified model of dark matter and dark energy. There is another unified model of a perfect fluid whose pressure is given by

$$P = -A\rho^{-\alpha}, \quad (10.105)$$

where ρ is the energy density, and α, A (> 0) are constants. If $\alpha = 1$, the above model is called the Chaplygin gas [63]. For general α , the model (10.105) is dubbed the generalized Chaplygin gas [64], whose equation of state is

$$w = -A\rho^{-\alpha-1}. \quad (10.106)$$

Substituting Eq. (10.105) into the continuity equation $\dot{\rho} + 3H(\rho + P) = 0$, we obtain the integrated solution

$$\rho = \left(A + \frac{B}{a^{3(1+\alpha)}} \right)^{1/(1+\alpha)}, \quad (10.107)$$

where B is a constant. Provided that $\alpha > -1$ and $B > 0$, we have $\rho \rightarrow \infty, w \rightarrow 0$ for $a \rightarrow 0$ and $\rho \rightarrow A^{1/(1+\alpha)}, w \rightarrow -1$ for $a \rightarrow \infty$. Hence the generalized Chaplygin gas shares the similar property as that in the k-essence model (10.98).

For the model (10.105), the sound speed squared is given by

$$c_s^2 = -\alpha w. \quad (10.108)$$

In the early matter era, w is close to 0, but the deviation from $w = 0$ starts to occur around the middle of the matter era to approach the final value $w = -1$. This means that $|c_s^2|$ also deviates from the initial value 0. For $c_s^2 > 0$, the pressure term $c_s^2 k^2/a^2$ prevents the gravitational attraction induced by the term $-4\pi G\rho$. For $c_s^2 < 0$, the pressure term works to enhance the gravitational attraction further. Unless the constant $|\alpha|$ is sufficiently small, the shape of the matter power spectrum is substantially modified. From the observed matter power spectrum, the parameter α was constrained to be [65]

$$|\alpha| \lesssim 10^{-5}, \quad (10.109)$$

which means that the Chaplygin gas model ($\alpha = 1$) is excluded. The bound (10.109) means that the generalized Chaplygin gas model (10.105) is hardly distinguished from the Λ CDM model ($P = -A$). The above results show that the information of the sound speed is crucially important for constraining the parameter space of unified models of dark energy and dark matter.

10.3. Coupled dark energy

Given the fact that the present Universe is dominated by two unknown dark components, there may be a possibility that dark energy and dark matter interact with each other. If the baryon is also coupled to dark energy, this gives rise to a long-range fifth force. Such a fifth force has not been experimentally observed, so it should be suppressed inside the solar system where local gravity experiments are carried out. On cosmological scales, there is a possibility that the baryon has an interaction with dark energy, but in such cases we need to resort to some screening mechanism to suppress the propagation of the fifth force in local regions of the Universe. Since the latter situation occurs in modified gravity theories, we will address the screening mechanism of interactions between baryons and dark energy in Chap. 14.

In this section, we study the cosmological dynamics of dark energy coupled to dark matter by neglecting the baryon contribution to non-relativistic matter. This is for the purpose of understanding how the coupling between dark energy and dark matter modifies the cosmological dynamics relative to the uncoupled case. In Sec. 11.2, we will study models in which both baryons and dark matter are coupled to dark energy in the context of Brans–Dicke theories.

On the FLRW background, the interaction between dark energy (energy–momentum tensor $T_{\nu(\text{DE})}^\mu$) and dark matter (energy–momentum tensor $T_{\nu(m)}^\mu$) may be written as

$$\nabla_\mu T^\mu_{\nu(\text{DE})} = -\beta, \quad (10.110)$$

$$\nabla_\mu T^\mu_{\nu(m)} = +\beta, \quad (10.111)$$

where β characterizes the interaction in the dark sector. The explicit form of β depends on underlying theories. One of the representative coupled dark energy scenarios with a scalar field ϕ is described by the interaction [66]

$$\beta = \frac{QT_m \nabla_\nu \phi}{M_{\text{pl}}}, \quad (10.112)$$

where Q is a dimensionless coupling, and T_m is the trace of the energy–momentum tensor $T_{\nu(m)}^\mu$ of the matter sector. For the perfect fluid with $T_{\nu(m)}^\mu = \text{diag}(-\rho, P, P, P)$ we have $T_m = -\rho + 3P$, so that $T_m \simeq -\rho$ for non-relativistic matter. Since the radiation is traceless, it does not couple to the scalar field. In

scalar–tensor theories, the coupling (10.112) arises after the conformal transformation to the Einstein frame [66, 67]. As we will discuss in Sec. 11.2, the coupling Q is constant [68, 69] in Brans–Dicke theories [70].

There are other phenomenological choices of couplings like $\beta = QH\rho_m$ and $\beta = Q\Omega_{\text{DE}}H$ [71–78]. However, it is generally difficult to motivate such couplings from some fundamental gravity or particle theories. There are some cases in which analytic expressions of the Hubble parameter can be known in terms of the redshift z by choosing specific forms of the coupling β , but we do not deal with such phenomenological cases in the following.

10.3.1. Coupled quintessence

We first study the background cosmological dynamics of coupled dark energy under the assumption that the coupling Q in Eq. (10.112) is constant. We consider a canonical scalar field ϕ with a potential $V(\phi)$, such that the system is described by the action

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} R - \frac{1}{2} g^{\mu\nu} \nabla_\mu \phi \nabla_\nu \phi - V(\phi) \right] + S_m(\phi) + S_r, \quad (10.113)$$

where S_m is the action of dark matter (energy density ρ_m) coupled to the dark energy field ϕ , and S_r is the action of radiation (energy density ρ_r) uncoupled to ϕ . On the flat FLRW background, the first Friedmann equation is

$$3M_{\text{pl}}^2 H^2 = \frac{1}{2} \dot{\phi}^2 + V(\phi) + \rho_m + \rho_r. \quad (10.114)$$

From the $\nu = 0$ components of Eqs. (10.110) and (10.111), we obtain

$$\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} = -\frac{Q\rho_m}{M_{\text{pl}}}, \quad (10.115)$$

$$\dot{\rho}_m + 3H\rho_m = \frac{Q\rho_m\dot{\phi}}{M_{\text{pl}}}. \quad (10.116)$$

The radiation obeys the standard continuity equation

$$\dot{\rho}_r + 4H\rho_r = 0. \quad (10.117)$$

Taking the time derivative of Eq. (10.114) and using Eqs. (10.115)–(10.117), it follows that

$$\frac{\dot{H}}{H^2} = -\frac{1}{2} (3 + 3x^2 - 3y^2 + \Omega_r), \quad (10.118)$$

where $\Omega_r \equiv \rho_r/(3M_{\text{pl}}^2 H^2)$, and the definitions of x and y are given by Eq. (10.7). Then, the effective equation of state $w_{\text{eff}} = -1 - 2\dot{H}/(3H^2)$ yields

$$w_{\text{eff}} = x^2 - y^2 + \frac{1}{3}\Omega_r, \quad (10.119)$$

with the field equation of state w_{DE} being the same as Eq. (10.8). We define the density parameters of the field and dark matter in the same way as Eq. (10.10), i.e.,

$$\Omega_\phi = x^2 + y^2, \quad \Omega_m \equiv \frac{\rho_m}{3M_{\text{pl}}^2 H^2} = 1 - x^2 - y^2 - \Omega_r. \quad (10.120)$$

The dimensionless variables x, y, Ω_r obey the differential equations

$$\frac{dx}{d\mathcal{N}} = -\frac{1}{2}x(3 - 3x^2 + 3y^2 - \Omega_r) + \frac{\sqrt{6}}{2}\lambda y^2 - \frac{\sqrt{6}}{2}Q(1 - x^2 - y^2 - \Omega_r), \quad (10.121)$$

$$\frac{dy}{d\mathcal{N}} = \frac{y}{2}(3 + 3x^2 - 3y^2 + \Omega_r - \sqrt{6}\lambda x), \quad (10.122)$$

$$\frac{d\Omega_r}{d\mathcal{N}} = \Omega_r(\Omega_r - 1 + 3x^2 - 3y^2). \quad (10.123)$$

In what follows, we study the background dynamics for the model with constant λ , i.e., for the exponential potential

$$V(\phi) = V_0 e^{-\lambda\phi/M_{\text{pl}}}. \quad (10.124)$$

The radiation-dominated fixed point of the above dynamical system corresponds to

$$(a) \quad (x, y, \Omega_r) = (0, 0, 1), \quad (10.125)$$

at which $\Omega_\phi = 0$, $\Omega_m = 0$, and $w_{\text{eff}} = 1/3$. Considering small perturbations $\delta x, \delta y, \delta\Omega_r$ around the point (a), the eigenvalues associated with the 3×3 Jacobian matrix of perturbations are $1, 2 - 1$, so the point (a) is a saddle.

In the presence of the coupling Q , the standard matter fixed point $(x, y, \Omega_r) = (0, 0, 0)$ does not exist, but it is replaced by

$$(b) \quad (x, y, \Omega_r) = \left(-\frac{\sqrt{6}}{3}Q, 0, 0\right). \quad (10.126)$$

This is called the ϕ -matter-dominated epoch (ϕMDE) [66], at which we have

$$\Omega_\phi = w_{\text{eff}} = \frac{2}{3}Q^2, \quad \Omega_m = 1 - \frac{2}{3}Q^2, \quad w_{\text{DE}} = 1. \quad (10.127)$$

Compared to the standard matter era, the field kinetic energy contributes to the total energy density through the coupling Q . The evolution of the scale factor during the ϕMDE is given by

$$a \propto t^{2/[3(1+w_{\text{eff}})]} = t^{2/(3+2Q^2)}. \quad (10.128)$$

Hence the existence of the coupling Q slows down the expansion rate of the Universe. The eigenvalues of the Jacobian matrix of homogeneous perturbations about the point (b) are $-3/2 + Q^2, -1/2 + Q^2, 3/2 + Q(Q + \lambda)$. As long as $Q^2 \ll 1$ and $\lambda \lesssim 1$, the fixed point (b) is a saddle with two negative eigenvalues.

The fixed point (c) derived in Table 10.1 for the uncoupled case, i.e.,

$$(c) \ (x, y, \Omega_r) = \left(\frac{\lambda}{\sqrt{6}}, \sqrt{1 - \frac{\lambda^2}{6}}, 0 \right), \quad (10.129)$$

is also present for $Q \neq 0$. At this point we have $\Omega_\phi = 1$ and $w_{\text{eff}} = w_{\text{DE}} = -1 + \lambda^2/3$, so the cosmic acceleration occurs for $\lambda^2 < 2$ (i.e., the same as the $Q = 0$ case). The eigenvalues of the Jacobian matrix of homogenous perturbations around the point (c) are $(\lambda^2 - 4)/2, (\lambda^2 - 6)/2, \lambda(Q + \lambda) - 3$. Under the condition $\lambda^2 < 2$, the point (c) is stable for

$$\lambda(Q + \lambda) < 3. \quad (10.130)$$

Provided that the two conditions (10.130) and $|Q| \ll 1$ are satisfied, the cosmological dynamics is given by the sequence of the fixed points: (a) $\rightarrow$ (b) $\rightarrow$ (c).

In Fig. 10.5, we plot the evolution of $w_{\text{eff}}, w_{\text{DE}}$ and $\Omega_\phi, \Omega_m, \Omega_r$ for $Q = 0.25$ and $\lambda = 0.2$. The radiation fixed point (a) is followed by the ϕ MDE satisfying $\Omega_\phi = w_{\text{eff}} = 2Q^2/3 \simeq 0.04$. Since the initial conditions of x and y are chosen to be $x \gg y$ in the radiation era, the field equation of state w_{DE} starts from the value close to 1 and stays with the value 1 during the ϕ MDE. After the end of

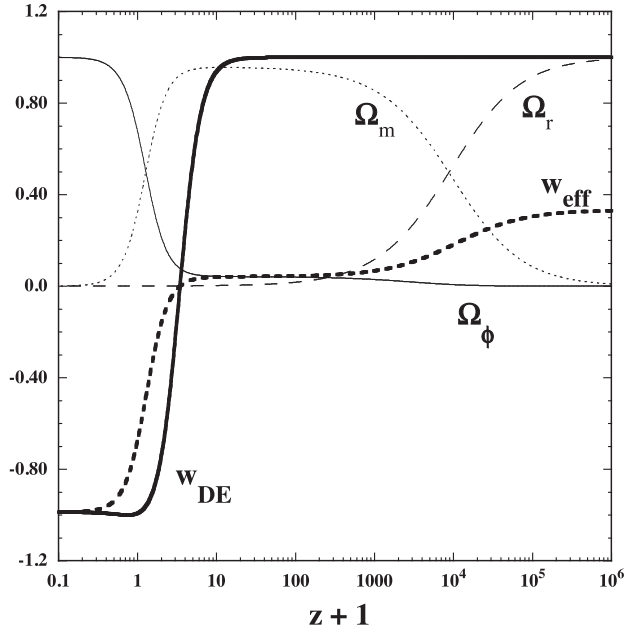


Fig. 10.5. Evolution of $w_{\text{eff}}, w_{\text{DE}}, \Omega_\phi, \Omega_m, \Omega_r$ versus $z+1$ for the coupled scalar-field dark energy model (10.113) with the exponential potential $V(\phi) = V_0 e^{-\lambda\phi/M_{\text{Pl}}}$. The model parameters are $Q = 0.25$ and $\lambda = 0.2$ with the initial conditions $x = 10^{-9}$, $y = 10^{-11}$, and $\Omega_r = 0.996$ at the redshift $z = 2.35 \times 10^6$. The present epoch ($z = 0$) is identified by $\Omega_\phi = 0.68$.

the ϕ MDE, the solution asymptotically approaches the fixed point (c) with $w_{\text{eff}} = w_{\text{DE}} = -1 + \lambda^2/3 \simeq -0.987$.

Existence of the coupling Q modifies the cosmological evolution from the last scattering surface to today. The CMB shift parameter $\mathcal{R}_{\text{CMB}}$ and the multipole l_A , defined by Eqs. (7.180) and (7.181) respectively, are affected by the existence of the ϕ MDE. The ϕ MDE corresponds to the kinetic scaling solution with $\Omega_\phi/\Omega_m = \text{constant}$, so it is not sensitive to the change of the field potential. The likelihood analysis using the WMAP7 data constrained the coupling to be $|Q| < 0.063$ (68% CL) for the inverse power-law potential $V(\phi) = V_0\phi^{-p}$ [79]. The joint analysis of Planck 2013, WMAP polarization, and BAO data for the same inverse power-law potential provided the bound $Q = 0.036 \pm 0.016$ at 68% CL [80]. Interestingly the non-zero coupling is compatible with the Planck CMB data, but the uncoupled case is within the 95% CL observational boundary.

The fixed point (b) is a kind of scaling solutions along which the ratio Ω_ϕ/Ω_m is a non-zero constant. Besides the fixed points (a), (b) and (c), there exists another scaling solution characterized by

$$(d) \ (x, y, \Omega_r) = \left(\frac{\sqrt{6}}{2(Q+\lambda)}, \sqrt{\frac{2Q(Q+\lambda)+3}{2(Q+\lambda)^2}}, 0 \right), \quad (10.131)$$

at which we have

$$\Omega_\phi = \frac{Q(Q+\lambda)+3}{(Q+\lambda)^2}, \quad w_{\text{DE}} = -\frac{Q(Q+\lambda)}{Q(Q+\lambda)+3}, \quad w_{\text{eff}} = -\frac{Q}{Q+\lambda}. \quad (10.132)$$

In the limit that $Q \rightarrow 0$, this recovers the scaling solution (d) in Table 10.1 with $w_m = 0$. For Q close to 0, we have $w_{\text{eff}} \simeq 0$, so the fixed point (10.131) cannot be used for the cosmic acceleration. If $|Q|$ is large such that the condition $Q/(Q+\lambda) > 1/3$ is satisfied, there is an interesting possibility that the scaling solution (10.131) is responsible for a global attractor with $\Omega_\phi \simeq 0.7$. The stability analysis around the point (d) shows that it can be a stable attractor for $\lambda(Q+\lambda) > 3$, i.e., the opposite inequality to Eq. (10.130) [81, 82]. To realize the accelerated scaling attractor, we require that the coupling $|Q|$ is large such that the conditions $Q/(Q+\lambda) > 1/3$ and $\lambda(Q+\lambda) > 3$ are satisfied, but we require the condition $Q^2 \ll 1$ for the existence of the ϕ MDE consistent with the CMB data. In fact, there are no allowed parameter spaces of Q and λ in which the transition from the ϕ MDE with $\Omega_\phi = 2Q^2/3 \ll 1$ to the scaling accelerated attractor with $\Omega_\phi \simeq 0.7$ can be realized [83].

In summary, the coupled dark energy model (10.113) with the exponential potential (10.124) gives rise to the cosmological sequence of the fixed points (a) $\rightarrow$ (b) $\rightarrow$ (c). Since the ϕ MDE is a kinetic fixed point, the bound on the coupling Q is not sensitive to the change of the scalar potential. In current CMB observations, the coupling $|Q|$ is constrained to be smaller than the order of 0.1. We need more accurate observational data to judge whether or not the non-zero coupling Q is favored over the uncoupled case.

10.3.2. Evolution of matter perturbations in coupled dark energy

In this section, we study the evolution of linear cosmological perturbations for the coupled dark energy scenario given by the action (10.113). Since we are interested in the dynamics of matter density perturbations associated with observations of large-scale structures and weak lensing, we do not take into account the contribution of radiation. We consider the perturbed metric (6.73) in the flat Universe with four scalar metric perturbations A, B, ψ, E with the cosmic time t , i.e.,

$$ds^2 = -(1 + 2A)dt^2 + 2aB_{|i}dtdx^i + a^2[(1 + 2\psi)\delta_{ij} + 2E_{|ij}]dx^i dx^j. \quad (10.133)$$

We fix the gauge after deriving the perturbation equations of motion. From Eqs. (6.57)–(6.59), the perturbations of energy density, momentum, and pressure for the scalar field with the Lagrangian $P = X - V(\phi)$ are given, respectively, by

$$\delta\rho_\phi = \dot{\phi}\delta\dot{\phi} - A\dot{\phi}^2 + V_{,\phi}\delta\phi, \quad \delta q_\phi = -\dot{\phi}\delta\phi, \quad \delta P_\phi = \dot{\phi}\delta\dot{\phi} - A\dot{\phi}^2 - V_{,\phi}\delta\phi, \quad (10.134)$$

where $\delta\phi$ is the perturbation of ϕ . We deal with dark matter as a perfect fluid with the density perturbation $\delta\rho_m$ and the momentum perturbation δq_m . At linear order, the $\nu = 0$ component of the coupling (10.112) is

$$\beta = -\frac{Q}{M_{\text{pl}}}(\rho_m\delta\dot{\phi} + \dot{\phi}\delta\rho_m). \quad (10.135)$$

On using Eq. (6.104), the $\nu = 0$ components of Eqs. (10.110) and (10.111) in Fourier space are given, respectively, by

$$\delta\dot{\rho}_\phi + 3H(\delta\rho_\phi + \delta P_\phi) + (\rho_\phi + P_\phi)\left(3\dot{\psi} - \frac{k^2}{a}\sigma\right) - \frac{k^2}{a^2}\delta q_\phi = -\frac{Q}{M_{\text{pl}}}(\rho_m\delta\dot{\phi} + \dot{\phi}\delta\rho_m), \quad (10.136)$$

$$\delta\dot{\rho}_m + 3H\delta\rho_m + \rho_m\left(3\dot{\psi} - \frac{k^2}{a}\sigma\right) - \frac{k^2}{a^2}\delta q_m = \frac{Q}{M_{\text{pl}}}(\rho_m\delta\dot{\phi} + \dot{\phi}\delta\rho_m), \quad (10.137)$$

where $\sigma = a\dot{E} - B$. The velocity potentials v_ϕ and v_m of the field and matter are related to their momentum perturbations, respectively, as $\delta q_\phi = a(\rho_\phi + P_\phi)(v_\phi + B)$ and $\delta q_m = a\rho_m(v_m + B)$. Employing the background equation (10.115), the $\nu = i$ component of Eq. (10.110) is automatically satisfied. On using Eq. (6.106), the $\nu = i$ component of Eq. (10.111) yields

$$\delta\dot{q}_m + 3H\delta q_m + \rho_m A = -\frac{Q}{M_{\text{pl}}}\rho_m\delta\phi. \quad (10.138)$$

The perturbed Einstein equations are given by

$$M_{\text{pl}}^2\delta G^\mu{}_\nu = \delta T^\mu{}_{\nu(\text{DE})} + \delta T^\mu{}_{\nu(m)}. \quad (10.139)$$

From the (00) and $i \neq j$ components, we obtain the perturbed equations of motion analogous to Eqs. (6.97) and (6.100), i.e.,

$$3H \left(\dot{\psi} - HA \right) + \frac{k^2}{a^2} \psi - \frac{H}{a} k^2 \sigma = \frac{1}{2M_{\text{pl}}^2} (\delta\rho_\phi + \delta\rho_m), \quad (10.140)$$

$$a(\dot{\sigma} + 2H\sigma) - A - \psi = 0, \quad (10.141)$$

where we used the fact that the anisotropic stress Π vanishes for both ϕ and the perfect fluid.

In the following, we choose the longitudinal gauge characterized by

$$B = E = 0, \quad (10.142)$$

under which $\sigma = 0$, and the gauge-invariant Bardeen potentials (6.63) and (6.64) reduce, respectively, to $\Psi = A$ and $\Phi = \psi$. We introduce the density contrast δ and the velocity potential $\mathcal{V}$ as

$$\delta \equiv \frac{\delta\rho_m}{\rho_m}, \quad \mathcal{V} \equiv -\frac{\delta q_m}{\rho_m}. \quad (10.143)$$

On using Eq. (10.134) and the background Eqs. (10.115) and (10.116), Eqs. (10.136)–(10.138), (10.140) and (10.141) can be expressed as

$$\ddot{\delta\phi} + 3H\dot{\delta\phi} + \left(\frac{k^2}{a^2} + m_\phi^2 \right) \delta\phi + 2\Psi V_{,\phi} + \dot{\phi} \left(3\dot{\Phi} - \dot{\Psi} \right) = -\frac{Q\rho_m}{M_{\text{pl}}} (\delta_m - 3H\mathcal{V} + 2\Psi), \quad (10.144)$$

$$\dot{\delta} + 3\dot{\Phi} + \frac{k^2}{a^2} \mathcal{V} = \frac{Q}{M_{\text{pl}}} \dot{\delta\phi}, \quad (10.145)$$

$$\dot{\mathcal{V}} - \Psi = \frac{Q}{M_{\text{pl}}} \left(\delta\phi - \dot{\phi}\mathcal{V} \right), \quad (10.146)$$

$$3H(\dot{\Phi} - H\Psi) + \frac{k^2}{a^2} \Phi = \frac{1}{2M_{\text{pl}}^2} [\delta\rho_\phi + \rho_m(\delta_m - 3H\mathcal{V})], \quad (10.147)$$

$$\Phi = -\Psi, \quad (10.148)$$

where $m_\phi^2 \equiv V_{,\phi\phi}$ is the mass squared of the scalar field, $\delta\rho_\phi = \dot{\phi}\dot{\delta\phi} - \Psi\dot{\phi}^2 + V_{,\phi}\delta\phi$, and δ_m is the gauge-invariant matter density contrast defined by

$$\delta_m \equiv \delta + 3H\mathcal{V}. \quad (10.149)$$

Taking the time derivative of Eq. (10.145) and using Eqs. (10.144) and (10.146), it follows that

$$\ddot{\delta}_m + \left(2H + \frac{Q\dot{\phi}}{M_{\text{pl}}} \right) \dot{\delta}_m + \frac{k^2}{a^2} \Psi + 3(\ddot{B} + 2H\dot{B})$$

$$\begin{aligned}
&= -\frac{Q}{M_{\text{pl}}} \left[\dot{\phi}(3\dot{\Phi} - \dot{\Psi}) + 3\dot{\phi}\dot{\mathcal{B}} + 2\Psi V_{,\phi} + \left(\frac{2k^2}{a^2} + m_\phi^2 \right) \delta\phi + \left(H - \frac{Q\dot{\phi}}{M_{\text{pl}}} \right) \delta\dot{\phi} \right. \\
&\quad \left. + \frac{Q\rho_m}{M_{\text{pl}}} (\delta_m - 3H\mathcal{V} + 2\Psi) \right], \tag{10.150}
\end{aligned}$$

where $\mathcal{B} \equiv \Phi - H\mathcal{V}$.

Since we are interested in testing for coupled dark energy with the observations of large-scale structures and weak lensing, we focus on the evolution of perturbations deep inside the Hubble radius ($k \gg aH$). From Eq. (10.145), the term $|H\mathcal{V}|$ is at most of the order of $(aH/k)^2 |\delta| \ll |\delta|$, so that $\delta_m \simeq \delta$ for sub-horizon modes. Ignoring the field density perturbation $\delta\rho_\phi$ relative to the matter density perturbation in Eq. (10.147), it follows that

$$\frac{k^2}{a^2} \Phi \simeq \frac{\rho_m}{2M_{\text{pl}}^2} \delta_m. \tag{10.151}$$

Using the matter density parameter $\Omega_m = \rho_m/(3M_{\text{pl}}^2 H^2)$, the relation (10.151) can be written as $\Phi \simeq 3\Omega_m \delta_m (aH/k)^2/2$. Hence $|\Phi|$ and $|\Psi|$ are much smaller than $|\delta_m|$ for $k \gg aH$.

The general solution to Eq. (10.144) can be expressed in terms of the sum of the homogeneous mode $\delta\phi_{\text{osc}}$ (derived by setting the right hand side to 0) and the special solution $\delta\phi_{\text{ind}}$ induced by the presence of the coupling Q , i.e.,

$$\delta\phi = \delta\phi_{\text{osc}} + \delta\phi_{\text{ind}}. \tag{10.152}$$

Neglecting the contributions of the gravitational potentials on the left hand side of Eq. (10.144), the homogeneous mode obeys

$$\delta\ddot{\phi}_{\text{osc}} + 3H\delta\dot{\phi}_{\text{osc}} + \left(\frac{k^2}{a^2} + m_\phi^2 \right) \delta\phi_{\text{osc}} \simeq 0. \tag{10.153}$$

The field mass m_ϕ is different depending on the form of the scalar potential. For the exponential potential $V(\phi) = V_0 e^{-\lambda\phi/M_{\text{pl}}}$ it follows that $m_\phi^2 = \lambda^2 V/M_{\text{pl}}^2 \approx \lambda^2 H^2 \Omega_\phi \lesssim \lambda^2 H^2$, where we used $\Omega_\phi \approx V/(H^2 M_{\text{pl}}^2)$. Since we require the condition $\lambda^2 < 2$ for the late-time cosmic acceleration, m_ϕ^2 is at most of the order of H^2 . In such cases, the term m_ϕ^2 in Eq. (10.153) can be neglected relative to k^2/a^2 . Introducing a rescaled field $\delta\varphi_{\text{osc}} = a\delta\phi_{\text{osc}}$, we can write Eq. (10.153) in the form

$$\delta\varphi_{\text{osc}}'' + \left(k^2 - \frac{a''}{a} \right) \delta\varphi_{\text{osc}} \simeq 0, \tag{10.154}$$

where a prime represents a derivative with respect to $\eta = \int a^{-1} dt$. The term a''/a is of the order of $(aH)^2$, so it can be neglected relative to k^2 for the modes deep

inside the Hubble radius. Then, the WKB solution to Eq. (10.154) is given by

$$\delta\phi_{\text{osc}} = \frac{\delta\varphi_{\text{osc}}}{a} \simeq \frac{1}{a\sqrt{2k}} (\alpha_k e^{-ik\eta} + \beta_k e^{ik\eta}), \quad (10.155)$$

where α_k and β_k are integration constants. The amplitude of $\delta\phi_{\text{osc}}$ decreases in proportion to a^{-1} .

The special solution $\delta\phi_{\text{ind}}$ corresponds to the one in which the term $(k^2/a^2)\delta\phi$ on the left hand side of Eq. (10.144) balances the coupling term on the right hand side, such that

$$\frac{k^2}{a^2}\delta\phi_{\text{ind}} \simeq -\frac{Q\rho_m}{M_{\text{pl}}}\delta_m. \quad (10.156)$$

In GR, the matter perturbation evolves as $\delta_m \propto a$ in the matter era, so the combination $a^2\rho_m\delta_m$ is constant. In coupled dark energy this property can be generally subject to change, but as long as $Q^2 \ll 1$, the variation of $\delta\phi_{\text{ind}}$ should be small relative to that of $\delta\phi_{\text{osc}}$. This means that, as long as the condition $|\delta\phi_{\text{ind}}| > |\delta\phi_{\text{osc}}|$ is initially satisfied, the oscillating mode $\delta\phi_{\text{osc}}$ should be negligible relative to the special solution $\delta\phi_{\text{ind}}$ induced by the coupling Q , i.e.,

$$\delta\phi \simeq \delta\phi_{\text{ind}} \simeq -\frac{a^2}{k^2} \frac{Q\rho_m}{M_{\text{pl}}}\delta_m. \quad (10.157)$$

This is the so-called quasi-static approximation under which time derivatives of the field perturbation $\delta\phi$ are dropped [84–86].

From Eqs. (10.148) and (10.151) we obtain the relation

$$\frac{k^2}{a^2}\Psi \simeq -\frac{\rho_m}{2M_{\text{pl}}^2}\delta_m, \quad (10.158)$$

which works as a source term for the growth of the matter density contrast δ_m on the left hand side of Eq. (10.150). Picking up dominant contributions in Eq. (10.150) for the perturbations deep inside the Hubble radius, it follows that

$$\ddot{\delta}_m + \left(2H + \frac{Q\dot{\phi}}{M_{\text{pl}}}\right)\dot{\delta}_m - \frac{\rho_m}{2M_{\text{pl}}^2}\delta_m \simeq -\frac{Q}{M_{\text{pl}}}\left(\frac{2k^2}{a^2}\delta\phi + \frac{Q\rho_m}{M_{\text{pl}}}\delta_m\right). \quad (10.159)$$

On the left hand side of Eq. (10.159), we did not ignore the term $Q\dot{\phi}/M_{\text{pl}} = \sqrt{6}QxH$ (where $x = \dot{\phi}/(\sqrt{6}HM_{\text{pl}})$), which is smaller than the order of H for $|Qx| \lesssim 1$. Substituting the solution (10.157) into Eq. (10.159), the matter density contrast obeys

$$\ddot{\delta}_m + \left(2H + \frac{Q\dot{\phi}}{M_{\text{pl}}}\right)\dot{\delta}_m - 4\pi G_{\text{eff}}\rho_m\delta_m \simeq 0, \quad (10.160)$$

where G_{eff} is the effective gravitational coupling given by [87]

$$G_{\text{eff}} = (1 + 2Q^2) G. \quad (10.161)$$

Existence of the coupling Q enhances the gravitational interaction with the matter perturbation. This leads to the larger growth rate of δ_m relative to that in the uncoupled case.

For example, we derive an analytic solution to δ_m during the ϕ MDE. In doing so, we rewrite Eq. (10.160) in terms of the derivative with respect to $\mathcal{N} = \ln a$, as

$$\frac{d^2\delta_m}{d\mathcal{N}^2} + \left(\frac{1}{2} - \frac{3}{2}w_{\text{eff}} + \sqrt{6}Qx\right) \frac{d\delta_m}{d\mathcal{N}} - \frac{3}{2}(1 + 2Q^2)\Omega_m\delta_m \simeq 0. \quad (10.162)$$

The ϕ MDE corresponds to $x = -\sqrt{6}Q/3$, $w_{\text{eff}} = 2Q^2/3$, and $\Omega_m = 1 - 2Q^2/3$, so the matter perturbation obeys

$$\frac{d^2\delta_m}{d\mathcal{N}^2} + \frac{1}{2}(1 - 6Q^2)\frac{d\delta_m}{d\mathcal{N}} - \frac{3}{2}(1 + 2Q^2)\left(1 - \frac{2}{3}Q^2\right)\delta_m \simeq 0. \quad (10.163)$$

The general solution to this equation is given by $\delta_m = c_1 e^{(1+2Q^2)\mathcal{N}} + c_2 e^{(-3/2+Q^2)\mathcal{N}}$, where c_1 and c_2 are integration constants. For $Q^2 \ll 1$, the latter corresponds to the decaying mode, so the matter perturbation grows as

$$\delta_m \propto a^{1+2Q^2} \propto t^{\frac{2+4Q^2}{3+2Q^2}}, \quad (10.164)$$

where we used $a \propto t^{2/(3+2Q^2)}$ during the ϕ MDE. Then, the matter growth rate is larger relative to the uncoupled case. During the ϕ MDE, the density parameter $\Omega_m = \rho_m/(3M_{\text{pl}}^2 H^2)$ is constant, so the matter density evolves as $\rho_m \propto H^2 \propto t^{-2} \propto a^{-3-2Q^2}$. From Eqs. (10.151) and (10.158), it then follows that

$$\Phi \simeq -\Psi = \text{constant}, \quad (10.165)$$

where its property is similar to the uncoupled case.

After the end of the ϕ MDE, it is not possible to obtain an analytic solution to Eq. (10.160). The gravitational potentials also start to vary after the onset of the cosmic acceleration. Solving the perturbation equations of motion numerically, it was shown in Ref. [88] that the growth rate $f \equiv \dot{\delta}_m/(H\delta_m)$ can be fitted by the formula

$$f = (\Omega_m)^\gamma (1 + \alpha Q^2), \quad (10.166)$$

where $\alpha \simeq 2.1$ and $\gamma \simeq 0.56$. On using this fitting formula, the coupling was constrained to be $|Q| < 0.52$ (95% CL) from the observational data of galaxy power spectra and Lyman- α forests. This is by one order of magnitude weaker than that derived from CMB. It is expected that future high-precision observations of redshift-space distortions like Euclid may provide tighter constraints on the coupling Q .

10.3.3. *Scaling k-essence Lagrangian and the coincidence problem*

As we discussed in Sec. 10.3.1, the ϕ MDE fixed point (b) corresponds to the scaling solution along which the ratio ρ_ϕ/ρ_m is a non-zero constant with $w_{\text{DE}} = 1$. For the canonical scalar field ϕ with the exponential potential, there is another scaling fixed point (d) with constant values of ρ_ϕ/ρ_m and w_{DE} . Since the analysis in Sec. 10.3.1 was restricted to be coupled quintessence, we are now interested in scaling solutions for more general scalar field models like k-essence. In this section, we derive an explicit form of the k-essence Lagrangian that allows the existence of scaling solutions.

In general, there is a so-called coincidence problem for dark energy and dark matter: why two dark components have roughly the same energy densities only recently in spite of the fact that they scale with time in different ways? To address this problem, we require that dark energy and dark matter follow the similar evolution with time, at least from some time onward. If there exists a scaling matter era with $\Omega_\phi/\Omega_m = \text{constant}$ followed by another accelerated scaling solution with $\Omega_\phi \approx 0.7$, this can alleviate the coincidence problem. We will study the possibility for realizing the sequence of two scaling solutions in k-essence.

Let us consider the k-essence scenario described by the action

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} R + P(\phi, X) \right] + S_m(\phi), \quad (10.167)$$

where the matter sector with the action S_m is coupled to the dark energy scalar field ϕ . We are interested in non-relativistic matter (dark matter) with the equation of state $w_m = 0$, but we keep w_m as an arbitrary constant in the following discussion. We assume that the coupling β is given by Eq. (10.112) with constant Q .

On the flat FLRW background, the continuity Eqs. (10.110) and (10.111) reduce, respectively, to

$$\dot{\rho}_\phi + 3H(1 + w_{\text{DE}})\rho_\phi = -\frac{Q\rho_m\dot{\phi}}{M_{\text{pl}}}, \quad (10.168)$$

$$\dot{\rho}_m + 3H(1 + w_m)\rho_m = \frac{Q\rho_m\dot{\phi}}{M_{\text{pl}}}, \quad (10.169)$$

where $\rho_\phi = 2XP_{,X} - P$ is the k-essence energy density with $w_{\text{DE}} = P/(2XP_{,X} - P)$, and ρ_m is the matter energy density. From the Friedmann equation, we have $3M_{\text{pl}}^2 H^2 = \rho_\phi + \rho_m$, so that

$$\Omega_\phi + \Omega_m = 1, \quad (10.170)$$

where $\Omega_\phi = \rho_\phi/(3M_{\text{pl}}^2 H^2)$ and $\Omega_m = \rho_m/(3M_{\text{pl}}^2 H^2)$. We search for scaling solutions along which the ratio ρ_ϕ/ρ_m and w_{DE} are constants. The former condition

translates to

$$\frac{\dot{\rho}_\phi}{\rho_\phi} = \frac{\dot{\rho}_m}{\rho_m}. \quad (10.171)$$

Using this relation in Eqs. (10.168) and (10.169), it follows that

$$\frac{d \ln \rho_\phi}{dt} = \frac{d \ln \rho_m}{dt} = -3H (1 + w_{\text{DE}} \Omega_\phi + w_m \Omega_m), \quad (10.172)$$

with

$$\frac{\dot{\phi}}{H} = \frac{3(w_m - w_{\text{DE}})M_{\text{pl}}\Omega_\phi}{Q} = \text{constant}. \quad (10.173)$$

Along the scaling solution the field equation of state $w_\phi = P/\rho_\phi$ is constant, so the field Lagrangian density P obeys the same form of equation as ρ_ϕ , i.e.,

$$\frac{d \ln P}{dt} = -3H (1 + w_{\text{DE}} \Omega_\phi + w_m \Omega_m). \quad (10.174)$$

Since P depends on ϕ and X , it follows that

$$\frac{\partial \ln P}{\partial \phi} \dot{\phi} + \frac{\partial \ln P}{\partial \ln X} \frac{d \ln X}{dt} = -3H (1 + w_{\text{DE}} \Omega_\phi + w_m \Omega_m). \quad (10.175)$$

From Eq. (10.173), the kinetic term has the dependence $X = \dot{\phi}^2/2 \propto H^2 \propto \rho_\phi$ for scaling solutions, so from Eq. (10.172) we obtain

$$\frac{d \ln X}{dt} = -3H (1 + w_{\text{DE}} \Omega_\phi + w_m \Omega_m). \quad (10.176)$$

Substituting Eqs. (10.173) and (10.176) into Eq. (10.175), the Lagrangian density P obeys the partial differential equation

$$\frac{\partial \ln P}{\partial \ln X} - \frac{M_{\text{pl}}}{\lambda} \frac{\partial \ln P}{\partial \phi} = 1, \quad (10.177)$$

where

$$\lambda \equiv Q \frac{1 + w_{\text{DE}} \Omega_\phi + w_m \Omega_m}{(w_m - w_{\text{DE}}) \Omega_\phi}. \quad (10.178)$$

The general solution to Eq. (10.177) is given by [59, 89]

$$P(\phi, X) = X g(Y), \quad Y \equiv X e^{\lambda \phi / M_{\text{pl}}}, \quad (10.179)$$

where g is an arbitrary function of Y . Thus we have shown that the existence of scaling solutions restricts the Lagrangian density in the form (10.179). While we derived the result (10.179) for the constant Q , it is possible to derive a more general form of the scaling Lagrangian for the coupling Q depending on the field ϕ [90].

The quintessence with an exponential potential, i.e., $P = X - V_0 e^{-\lambda\phi/M_{\text{pl}}}$, corresponds to the choice $g(Y) = 1 - V_0/Y$. For the choice $g(Y) = -1 + Y/M^4$ we recover the dilatonic ghost condensate model with $P = -X + e^{\lambda\phi/M_{\text{pl}}} X^2/M^4$, so this model also has scaling solutions.

The Lagrangian density (10.179) can be written in a different form. Introducing a rescaled field $\varphi = e^{\beta\lambda\phi/M_{\text{pl}}} M_{\text{pl}}/(\beta\lambda)$, where β is a constant, the kinetic energy $\tilde{X} = -(1/2)g^{\mu\nu}\nabla_\mu\varphi\nabla_\nu\varphi$ of the field φ is related to X , as $X = \tilde{X}e^{-2\beta\lambda\phi/M_{\text{pl}}}$. Since the quantity $Y = Xe^{\lambda\phi/M_{\text{pl}}}$ is expressed as $Y = \tilde{X}(\beta\lambda\varphi/M_{\text{pl}})^{(1-2\beta)/\beta}$, we have $Y = \tilde{X}$ for $\beta = 1/2$. Then, under the transformation $\varphi = 2e^{\lambda\phi/(2M_{\text{pl}})} M_{\text{pl}}/\lambda$, the scaling Lagrangian density (10.179) can be expressed as [55]

$$P(\varphi, \tilde{X}) = V(\varphi)f(\tilde{X}), \quad (10.180)$$

where

$$V(\varphi) = \left(\frac{\lambda\varphi}{2M_{\text{pl}}} \right)^{-2}, \quad f(\tilde{X}) = \tilde{X}g(\tilde{X}). \quad (10.181)$$

The Lagrangian density (10.69) of the tachyon field φ is given by $P = -V(\varphi)\sqrt{1-2\tilde{X}}$. Hence the tachyon with the potential $V(\varphi) \propto \varphi^{-2}$ has scaling solutions [53, 54].

We study the cosmological dynamics for the scaling Lagrangian density (10.179) in the presence of dark matter (equation of state $w_m = 0$) coupled to the k-essence field. Since we are interested in the cosmological dynamics after the onset of the matter era, we do not take into account the contribution of radiation. We also use the unit $M_{\text{pl}}^2 = 1$ and assume that $\lambda > 0$ in the following discussion. To derive the fixed points of the system, it is convenient to introduce the dimensionless variables:

$$x \equiv \frac{\dot{\phi}}{\sqrt{6}H}, \quad y \equiv \frac{e^{-\lambda\phi/2}}{\sqrt{3}H}, \quad (10.182)$$

with which the quantity $Y = Xe^{\lambda\phi}$ can be expressed as $Y = x^2/y^2$. On the flat FLRW background, the dynamical equations of motion are given by Eqs. (10.168)–(10.170) with $P_\phi = Xg$ and $\rho_\phi = X(g + 2Yg_Y)$. Then, we obtain the autonomous equations [82, 90]

$$\begin{aligned} \frac{dx}{dN} &= \frac{3x}{2} [1 + gx^2 - 2A(g + g_1)] \\ &+ \frac{\sqrt{6}}{2} [x^2\{A(Q + \lambda)(g + 2g_1) - \lambda\} - QA], \end{aligned} \quad (10.183)$$

$$\frac{dy}{dN} = \frac{y}{2} (3 - \sqrt{6}\lambda x + 3gx^2), \quad (10.184)$$

where $g_n \equiv Y^n \partial^n g / \partial Y^n$ and $A(Y) \equiv (g + 5g_1 + 2g_2)^{-1}$. Since the quantity A is related to the field sound speed squared c_s^2 as $c_s^2 = AP_{,X}$, we require that

$$A > 0, \quad P_{,X} = g + g_1 > 0 \quad (10.185)$$

to avoid the ghost and the Laplacian instability. The field equation of state, the effective equation of state, and the field density parameter are given, respectively, by

$$w_{\text{DE}} = \frac{g}{g + 2g_1}, \quad w_{\text{eff}} = gx^2, \quad \Omega_\phi = x^2 (g + 2g_1) = \frac{w_{\text{eff}}}{w_{\text{DE}}}. \quad (10.186)$$

We focus on the situation in which the field density parameter is in the range $0 \leq \Omega_\phi \leq 1$.

From Eq. (10.184), there are fixed points satisfying $3 - \sqrt{6}\lambda x + 3gx^2 = 0$, i.e.,

$$x = \frac{\sqrt{6}(1 + w_{\text{eff}})}{2\lambda}. \quad (10.187)$$

Substituting Eq. (10.187) and the relations $g_1 = (\Omega_\phi/x^2 - g)/2$ and $g = w_{\text{eff}}/x^2$ into Eq. (10.183), it follows that

$$\frac{dx}{dN} = \frac{\sqrt{6}A}{2(1 + w_{\text{eff}})}(\Omega_\phi - 1)[(Q + \lambda)w_{\text{eff}} + Q]. \quad (10.188)$$

For $w_{\text{eff}} \neq -1$ and $A \neq 0$, there are two fixed points characterized by (A) $\Omega_\phi = 1$ and (B) $w_{\text{eff}} = -Q/(Q + \lambda)$, i.e.,

(A) Scalar-field dominated solution

$$x_A = \frac{\lambda}{\sqrt{6}P_{,X}}, \quad \Omega_\phi = 1, \quad w_{\text{eff}} = w_{\text{DE}} = -1 + \frac{\lambda^2}{3P_{,X}}. \quad (10.189)$$

(B) Scaling solution

$$\begin{aligned} x_B &= \frac{\sqrt{6}}{2(Q + \lambda)}, & \Omega_\phi &= \frac{Q(Q + \lambda) + 3P_{,X}}{(Q + \lambda)^2}, \\ w_{\text{eff}} &= -\frac{Q}{Q + \lambda}, & w_{\text{DE}} &= -\frac{Q(Q + \lambda)}{Q(Q + \lambda) + 3P_{,X}}. \end{aligned} \quad (10.190)$$

For quintessence with the exponential potential ($P_{,X} = 1$), the points (A) and (B) correspond to the fixed points (c) and (d), respectively, derived in Table 10.1 of Sec. 10.3.1. The point (A) is responsible for the cosmic acceleration for $\lambda^2/P_{,X} < 2$. Provided that $Q > \lambda/2 > 0$ or $Q < -\lambda < 0$, it is also possible for the point (B) to lead to the cosmic acceleration.

The stability of the fixed points is known by perturbing Eqs. (10.183)–(10.184) about them and computing eigenvalues of the 2×2 Jacobian matrix for the perturbations δx and δy . The two eigenvalues for the points (A) and (B) are given, respectively, by

$$(A) \quad \mu_1 = -3 + \frac{\lambda(Q + \lambda)}{P_{,X}}, \quad \mu_2 = -3 + \frac{\lambda^2}{2P_{,X}}, \quad (10.191)$$

$$(B) \quad \mu_{\pm} = -\frac{3(2Q + \lambda)}{4(Q + \lambda)} \left[1 \pm \sqrt{1 - \frac{8(1 - \Omega_{\phi})(Q + \lambda)^3 [\Omega_{\phi}(Q + \lambda) + Q]}{3(2Q + \lambda)^2}} A \right]. \quad (10.192)$$

If the point (A) is responsible for the cosmic acceleration, we require that $w_{\text{eff}} = -1 + \lambda^2/(3P_{,X}) < -1/3$, i.e., $\lambda^2/P_{,X} < 2$, in which case μ_2 is negative. Then, the point (A) is stable under the condition

$$3P_{,X} > \lambda(Q + \lambda). \quad (10.193)$$

The point (B) leads to the cosmic acceleration for $Q > \lambda/2 > 0$ or $Q < -\lambda < 0$, under which the point (B) is stable if $-Q/(Q + \lambda) \leq \Omega_{\phi} < 1$. Since the left inequality is automatically satisfied for $\Omega_{\phi} \geq 0$, the stability of the point (B) with the cosmic acceleration is ensured for

$$3P_{,X} < \lambda(Q + \lambda). \quad (10.194)$$

The inequality (10.194) is opposite to the stability condition (10.193) of the point (A). This means that, if the point (B) is stable, then the point (A) is unstable [82]. In other words, the solutions choose either the point (A) or the point (B) as an accelerated attractor, depending on the values of Q and λ . The scaling solution (B) can be responsible for the cosmic acceleration only when the coupling $|Q|$ is larger than the order of λ .

There exist other fixed points satisfying $y = 0$ in Eq. (10.184). The ϕ MDE derived in Sec. 10.3.1 belongs to one of such fixed points. Since the quantity Y is expressed as $Y = x^2/y^2$, the function $g(Y)$ cannot be singular at $y = 0$ for the existence of the ϕ MDE. Then, the function $g(Y)$ should be expanded in negative powers of Y , i.e.,

$$g(Y) = c_0 + \sum_{n>0} c_n Y^{-n} = c_0 + \sum_{n>0} c_n \left(\frac{y^2}{x^2} \right)^n, \quad (10.195)$$

which includes quintessence with the exponential potential. For the function $g(Y)$ of the form (10.195), there exists the ϕ MDE fixed point satisfying

$$(C) \quad (x_C, y_C) = \left(-\frac{\sqrt{6}Q}{3c_0}, 0 \right), \quad \Omega_{\phi} = w_{\text{eff}} = \frac{2Q^2}{3c_0}, \quad w_{\text{DE}} = 1. \quad (10.196)$$

For $c_0 > 0$, we also have the purely kinetic point (D): $(x_D, y_D) = (\pm 1/\sqrt{c_0}, 0)$ with $\Omega_\phi = 1$.

If the ϕ MDE fixed point (C) is followed by another accelerated scaling solution (B) with $\Omega_\phi \approx 0.7$, this can alleviate the coincidence problem because the ratio Ω_ϕ/Ω_m remains constant during both ϕ MDE and the accelerated epoch. We consider the function (10.195) with $c_0 > 0$, under which Ω_ϕ for the point (C) is positive. The fixed point (B) can lead to the cosmic acceleration for (i) $Q > \lambda/2 > 0$, or (ii) $Q < -\lambda < 0$. In the case (i), x_B is positive, whereas x_C is negative. In the case (ii), x_B is negative, whereas x_C is positive. In both cases, the signs of x_B and x_C are different from each other. To realize the transition from (C) to (B), the solutions need to cross the line $x = 0$ in the (x, y) plane.

We consider the theory described by the single power-law function

$$g(Y) = c_0 - c_p Y^{-p}, \quad (10.197)$$

where $p \geq 1$. For this theory, the quantity A reduces to $A = Y^p/[c_0 Y^p - c_p(p-1)(2p-1)]$. At $x = 0$, we have $A = 0$ for $p \neq 1$ and $A = 1/c_0$ for $p = 1$. In the former case, the terms on the right hand side of Eqs. (10.183) and (10.184) yield $dx/d\mathcal{N} \rightarrow 0$ and $dy/d\mathcal{N} \rightarrow 3y/2$ as $x \rightarrow 0$, so the derivative dy/dx diverges when the solutions cross the line $x = 0$ with $y \neq 0$. Hence the point (C) is disconnected to the point (B) due to the divergence of the derivative dy/dx at $x = 0$. For $p = 1$, i.e., quintessence with the exponential potential, the singularity on the line $x = 0$ is absent, but it was shown in Ref. [66] that the conditions $\Omega_\phi < 0.7 \pm 0.2$, $w_{\text{eff}}^{(\text{B})} < -0.6 \pm 0.2$ at the point (B) (required for the cosmic acceleration) and the condition $\Omega_\phi < 0.2$ at the point (C) (required for the consistency with CMB measurements) are not simultaneously satisfied.

The above discussion shows that it is generally difficult to address the coincidence problem even for the general Lagrangian (10.179) with two scaling solutions. This problem intrinsically comes from the fact that a large coupling Q required for the existence of the scaling solution (B) with $\Omega_\phi \approx 0.7$ is not compatible with a small coupling Q required for the existence of the viable ϕ MDE ($\Omega_\phi \ll 1$). To realize such a transition, we need a time-varying coupling Q that rapidly grows from a small value to a large value [83]. However, it is difficult to theoretically motivate the origin of such fast varying couplings.

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Chapter 11

Modified Gravity Models of Dark Energy

The second approach to the problem of the late-time cosmic acceleration is based on the modification of gravity at large distances. The left hand side of Einstein equations (3.85) is modified in this approach. In terms of the action (3.87), the Lagrangian density R is subject to change. This geometric modification breaks the gauge symmetry of GR, which generally gives rise to additional propagating degrees of freedom. It is possible to construct models in which the new degrees of freedom give rise to the cosmic acceleration. In this chapter, we introduce several representative models of modified gravity with a *scalar* degree of freedom and study the resulting background cosmological dynamics. In Chap. 12, we consider more general theories with second-order equations of motion and study the evolution of cosmological perturbations and their observational consequences. These theories need to recover the gravitational law close to that of GR in the solar system for the consistency with local gravity experiments. In Chap. 14, we will discuss several mechanisms of how to screen fifth forces mediated by new dynamical degrees of freedom.

11.1. $f(R)$ gravity

The simplest modification to GR arises from the change of the Ricci scalar R in the gravitational action [1–3]. Let us consider $f(R)$ theories given by the action [4, 5]

$$S = \frac{M_{\text{pl}}^2}{2} \int d^4x \sqrt{-g} f(R) + \int d^4x L_m(g_{\mu\nu}, \Psi_m), \quad (11.1)$$

where f is a function of R , and L_m is the Lagrangian of matter fields Ψ_m . We assume that matter is minimally coupled to gravity. In the standard variational approach called the metric formalism, the action (11.1) is varied with respect to the metric $g_{\mu\nu}$ by dealing with the affine connections $\Gamma_{\beta\gamma}^\alpha$ as independent variables. There is

another way for the variation of the action called the Palatini formalism [6] in which $\Gamma_{\beta\gamma}^\alpha$ and $g_{\mu\nu}$ are treated as independent variables. In the context of $f(R)$ gravity, however, the Palatini variation of the action (11.1) leads to the strong coupling problem where the coupling between matter and the gravity sector is infinitely large [7–10]. In the following, we focus on the metric variational approach.

Varying the action (11.1) with respect to the metric, it follows that

$$\delta S = \frac{M_{\text{pl}}^2}{2} \int d^4x \left[\delta(\sqrt{-g})f(R) + \sqrt{-g}f_{,R}(R)\delta R - \frac{1}{M_{\text{pl}}^2} \sqrt{-g} T_{\mu\nu}^{(m)} \delta g^{\mu\nu} \right], \quad (11.2)$$

where $f_{,R} = \partial f / \partial R$, and $T_{\mu\nu}^{(m)} = -(2/\sqrt{-g})\delta L_m / \delta g^{\mu\nu}$ is the energy–momentum tensor of matter. The first term inside the square bracket of Eq. (11.2) can be computed from Eq. (3.95). For the computation of δR , we start with the variation of the Ricci tensor which is given by the following property:

$$\delta R_{\mu\nu} = \nabla_\rho \delta \Gamma_{\mu\nu}^\rho - \nabla_\mu \delta \Gamma_{\nu\rho}^\rho. \quad (11.3)$$

Since the relations $g^{\mu\nu} \nabla_\rho \delta \Gamma_{\mu\nu}^\rho = (-\delta_\mu^\beta \delta_\nu^\alpha + g_{\mu\nu} g^{\alpha\beta} / 2) \nabla_\alpha \nabla_\beta \delta g^{\mu\nu}$ and $g^{\mu\nu} \nabla_\mu \delta \Gamma_{\nu\rho}^\rho = -(1/2) g^{\alpha\beta} g_{\mu\nu} \nabla_\alpha \nabla_\beta \delta g^{\mu\nu}$ hold, it follows that

$$g^{\mu\nu} \delta R_{\mu\nu} = (-\delta_\mu^\beta \delta_\nu^\alpha + g_{\mu\nu} g^{\alpha\beta}) \nabla_\alpha \nabla_\beta \delta g^{\mu\nu}. \quad (11.4)$$

Hence the variation of the Ricci scalar $R = g^{\mu\nu} R_{\mu\nu}$ is given by

$$\delta R = R_{\mu\nu} \delta g^{\mu\nu} + (-\delta_\mu^\beta \delta_\nu^\alpha + g_{\mu\nu} g^{\alpha\beta}) \nabla_\alpha \nabla_\beta \delta g^{\mu\nu}. \quad (11.5)$$

Substituting Eqs. (3.95) and (11.5) into Eq. (11.2) and integrating the action twice by parts, we obtain

$$\delta S = \frac{M_{\text{pl}}^2}{2} \int d^4x \sqrt{-g} \left(-\frac{1}{2} f g_{\mu\nu} + f_{,R} R_{\mu\nu} - \nabla_\mu \nabla_\nu f_{,R} + g_{\mu\nu} \square f_{,R} - \frac{T_{\mu\nu}^{(m)}}{M_{\text{pl}}^2} \right) \delta g^{\mu\nu}, \quad (11.6)$$

where $\square \equiv g^{\alpha\beta} \nabla_\alpha \nabla_\beta$. Hence the variational principle ($\delta S / \delta g^{\mu\nu} = 0$) leads to the gravitational equations of motion

$$f_{,R} R_{\mu\nu} - \frac{1}{2} f g_{\mu\nu} - \nabla_\mu \nabla_\nu f_{,R} + g_{\mu\nu} \square f_{,R} = \frac{T_{\mu\nu}^{(m)}}{M_{\text{pl}}^2}. \quad (11.7)$$

If the function $f(R)$ contains non-linear terms in R , the third and fourth terms on the left hand side of Eq. (11.7) do not vanish. Since they contain the second derivatives, the term $\phi \equiv f_{,R}$ works as a propagating degree of freedom arising beyond the domain of GR. The quantity ϕ behaves as a scalar field with the gravitational

origin, which is called a scalaron [11]. Thus, $f(R)$ gravity gives rise to an additional scalar degree of freedom to that in GR. Taking the trace of Eq. (11.7), we obtain

$$3\Box f_{,R} + f_{,R}R - 2f = \frac{T_m}{M_{\text{pl}}^2}. \quad (11.8)$$

The trace of matter is given by $T_m = g^{\mu\nu}T_{\mu\nu}^{(m)} = -\rho_m + 3P_m$, where ρ_m and P_m are the energy density and the pressure, respectively.

If there exists a de Sitter vacuum solution on the flat FLRW background, then the Hubble expansion rate is constant and hence the Ricci scalar $R = 6(2H^2 + \dot{H})$ is constant. Since $\Box f_{,R} = 0$ at this point, we obtain

$$f_{,R}R - 2f = 0. \quad (11.9)$$

The function $f(R) = \alpha R^2$ (α is constant) satisfies the condition (11.9), so this model gives rise to an exact de Sitter solution. The first model of inflation proposed by Starobinsky [11] corresponds to $f(R) = R + \alpha R^2$, in which case the cosmic acceleration ends when the term αR^2 drops below R . Since R^2 decreases faster than R after inflation, the model $f(R) = R + \alpha R^2$ cannot be used for the late-time cosmic acceleration.

To construct viable $f(R)$ dark energy models, there are several conditions to be satisfied. If the modification from GR is large in the radiation and early matter eras, then the model can contradict with observations like CMB. Hence the viable models should be constructed to recover the behavior close to GR, i.e.,

$$f(R) = R - 2\Lambda \quad \text{for } R \gg R_0, \quad (11.10)$$

where Λ and R_0 are constants which are at most of the order of H_0^2 . The deviation from GR can occur at a late cosmological epoch. If we demand the existence of a de Sitter solution responsible for the cosmic acceleration, the function $f(R)$ needs to satisfy the condition (11.9) at the de Sitter fixed point.

In Sec. 12.4.1, we will derive theoretically consistent conditions of $f(R)$ gravity by studying cosmological perturbations on the flat FLRW background. The ghosts associated with tensor and scalar perturbations do not arise for

$$f_{,R} > 0. \quad (11.11)$$

In Sec. 12.4.1, we will show that the mass squared appearing in the perturbation equation of the scalaron perturbation is given by

$$M^2 = \frac{1}{3} \left(\frac{f_{,R}}{f_{,RR}} - R \right). \quad (11.12)$$

In the early Universe, the function $f(R)$ should be close to Eq. (11.10), so the dominant contribution to M^2 is the term $f_{,R}/(3f_{,RR})$. To avoid the tachyonic instability

of perturbations arising from negative M^2 , we require that

$$f_{,RR} > 0, \quad (11.13)$$

in addition to the condition (11.11). The model with the function $f(R) = R - \alpha/R^p$ ($\alpha > 0, p > 0$), which corresponds to the first $f(R)$ model of dark energy [12–15], gives the negative value $f_{,RR} = -\alpha p(p+1)R^{-p-2} < 0$, so it does not satisfy the condition (11.13).

The examples of viable dark energy models satisfying the above requirements are [16–18]

$$(i) \quad f(R) = R - \lambda R_0 \frac{(R/R_0)^{2n}}{(R/R_0)^{2n} + 1}, \quad (11.14)$$

$$(ii) \quad f(R) = R - \lambda R_0 \left[1 - \left(1 + \frac{R^2}{R_0^2} \right)^{-n} \right], \quad (11.15)$$

$$(iii) \quad f(R) = R - \lambda R_0 \tanh \left(\frac{R}{R_0} \right), \quad (11.16)$$

where λ , R_0 , and n are positive constants (see Refs. [19, 20] for other viable models). All these models satisfy the condition $f(R=0) = 0$, so the cosmological constant vanishes in the limit of the flat spacetime. In the regime $R \gg R_0$, the models (i) and (ii) have the asymptotic behavior

$$f(R) \simeq R - \lambda R_0 \left[1 - \left(\frac{R_0}{R} \right)^{2n} \right]. \quad (11.17)$$

In the model (iii), the approach to $f(R) = R - \lambda R_0$ occurs even faster with the growth of R . In the above models, the deviation from GR becomes important after R decreases to the order of R_0 .

We study the background cosmological dynamics for the viable $f(R)$ models presented above. In doing so, we first derive autonomous equations of motion without restricting the functional form of $f(R)$ and discuss conditions for the stability of (instantaneous) fixed points. We are interested in the cosmological evolution after the end of the radiation era, so we take into account non-relativistic matter with the energy density ρ_m and the negligible pressure in the action (11.1). On the flat FLRW spacetime with the line element $ds^2 = -dt^2 + a^2(t)\delta_{ij}dx^i dx^j$, the background equations of motion following from Eq. (11.7) are given by

$$3M_{\text{pl}}^2 f_{,R} H^2 = \rho_m + \frac{M_{\text{pl}}^2}{2} (f_{,RR} \dot{R} - \dot{f}) - 3M_{\text{pl}}^2 H \dot{f}_{,R}, \quad (11.18)$$

$$2M_{\text{pl}}^2 f_{,R} \dot{H} = -\rho_m + M_{\text{pl}}^2 \left(H \dot{f}_{,R} - \ddot{f}_{,R} \right), \quad (11.19)$$

together with the continuity equation $\dot{\rho}_m + 3H\rho_m = 0$. We introduce the dimensionless quantities [21]

$$x_1 \equiv -\frac{\dot{f}_{,R}}{Hf_{,R}}, \quad x_2 \equiv -\frac{f}{6f_{,R}H^2}, \quad x_3 \equiv \frac{R}{6H^2}, \quad m \equiv \frac{Rf_{,RR}}{f_{,R}}, \quad (11.20)$$

and the density parameters

$$\Omega_m \equiv \frac{\rho_m}{3M_{\text{pl}}^2 f_{,R} H^2} = 1 - x_1 - x_2 - x_3, \quad \Omega_{\text{DE}} \equiv x_1 + x_2 + x_3. \quad (11.21)$$

The effective equation of the system is given by $w_{\text{eff}} = (1 - 2x_3)/3$. Then, we obtain the following dynamical equations

$$\frac{dx_1}{d\mathcal{N}} = -1 - x_3 - 3x_2 + x_1^2 - x_1x_3, \quad (11.22)$$

$$\frac{dx_2}{d\mathcal{N}} = \frac{x_1x_3}{m} - x_2(2x_3 - 4 - x_1), \quad (11.23)$$

$$\frac{dx_3}{d\mathcal{N}} = -\frac{x_1x_3}{m} - 2x_3(x_3 - 2), \quad (11.24)$$

where $\mathcal{N} = \ln a$. The quantity m , which characterizes the deviation from GR, is a function of R . Defining another variable

$$r \equiv -\frac{Rf_{,R}}{f} = \frac{x_3}{x_2}, \quad (11.25)$$

the quantity m is a function of r . The cosmological dynamics can be viewed as the trajectories in the (m, r) plane. Provided that the variation of m is small over cosmological time scales, we can derive instantaneous fixed points of the above dynamical system by dealing with m as constants [21]. The instantaneous fixed point relevant to the matter-dominated epoch is given by

$$(A) \ (x_1, x_2, x_3) = \left(\frac{3m}{1+m}, -\frac{1+4m}{2(1+m)^2}, \frac{1+4m}{2(1+m)} \right), \quad (11.26)$$

at which $r = -1$, $w_{\text{eff}} = -m/(1+m)$ and $\Omega_m = 1 - m(7+10m)/[2(1+m)^2]$. Provided that $|m| \ll 1$, we have $w_{\text{eff}} \simeq 0$ and $\Omega_m \simeq 1$ at the point (A), so it can be responsible for the matter-dominated era. The de Sitter fixed point satisfying the condition (11.9) corresponds to

$$(B) \ (x_1, x_2, x_3) = (0, -1, 2), \quad (11.27)$$

at which $r = -2$, $w_{\text{eff}} = -1$ and $\Omega_m = 0$. In the (m, r) plane, the cosmological trajectories evolve from the matter point (A) close to $(m, r) = (0, -1)$ toward the de Sitter point (B) on the line $r = -2$ with non-zero m .

Considering homogenous perturbations around the point (A), the eigenvalues of the 3×3 Jacobian matrix are given by

$$\frac{-3m \pm \sqrt{m(256m^3 + 160m^2 - 31m - 16)}}{4m(m+1)}, \quad 3 \left(1 + \frac{dm}{dr}\right). \quad (11.28)$$

In the limit that $|m| \ll 1$, the first two eigenvalues reduce to $-3/4 \pm \sqrt{-1/m}$. For the models with $m < 0$, one of the eigenvalues diverges as $m \rightarrow -0$, so the solutions cannot remain for a long time around the point (A). This is the reason why the model $f(R) = R - \alpha/R^p$ ($\alpha > 0, p > 0$), in which $f_{,RR} < 0$ and $f_{,R} > 0$, does not have a proper matter era [22].

On the other hand, for $m > 0$, the latter two eigenvalues in Eq. (11.28) are complex with negative real parts. Provided that $dm/dr > -1$, the point (A) is a saddle point with a damped oscillation of homogenous perturbations. Then, the solutions stay around this point for some period and finally leave there for approaching another stable fixed point relevant to the cosmic acceleration. Hence the conditions for the existence of the saddle matter era yield

$$m(r = -1) \simeq +0, \quad \frac{dm}{dr}(r = -1) > -1. \quad (11.29)$$

We note that the positivity of the quantity $m = Rf_{,RR}/f_{,R}$ is also consistent with the conditions (11.11) and (11.13) for $R > 0$. Let us apply the conditions (11.29) to the models (i) and (ii) in the regime $R \gg R_0$. On using the asymptotic form of $f(R)$ given by Eq. (11.17), the quantities m and r approximately reduce to $m \simeq 2\lambda n(1+2n)(R_0/R)^{1+2n}$ and $r \simeq -R/(R - \lambda R_0)$. Then, it follows that

$$m(r) \simeq 2\lambda n(1+2n) \left(-\frac{r+1}{\lambda}\right)^{1+2n}, \quad \frac{dm}{dr}(r) \simeq -2n(1+2n)^2 \left(-\frac{r+1}{\lambda}\right)^{2n}. \quad (11.30)$$

For $R \gg R_0$, the quantity r is sufficiently close to -1 (i.e., $r = -1 - \epsilon$ with $0 < \epsilon \ll 1$), so the conditions (11.29) are well satisfied.

The eigenvalues of the Jacobian matrix of homogenous perturbations about the point (B) are given by

$$-\frac{3}{2} \pm \frac{\sqrt{25 - 16/m}}{2}, \quad -3. \quad (11.31)$$

Hence the stability of the de Sitter point requires that [21, 23, 24]

$$0 < m(r = -2) \leq 1. \quad (11.32)$$

The conditions (11.29) and (11.32) can be generally satisfied for the models in which the parameter m remains smaller than the order of 1 during the transition from the point (A) to the point (B).

Existence and stability of the de Sitter fixed point (B) restricts the parameter space of viable $f(R)$ models of dark energy. For the model (i), there is the following relation from Eq. (11.9):

$$\lambda = \frac{(1 + x_1^{2n})^2}{x_1^{2n-1}(2 + 2x_1^{2n} - 2n)}, \quad (11.33)$$

where R_1 is the value of R at the de Sitter point, and $x_1 \equiv R_1/R_0$. The stability condition (11.32) gives

$$2x_1^{4n} - 2(n+2)(2n-1)x_1^{2n} + (2n-1)(2n-2) \geq 0. \quad (11.34)$$

For given n , the condition (11.34) provides a lower bound on the parameter λ . If $n = 1$, we have $x_1 \geq \sqrt{3}$ and $\lambda \geq 8\sqrt{3}/9$. Under the inequality (11.34), we can show that the conditions (11.11) and (11.13) are also satisfied for $R \geq R_1$.

For the model (ii), the stability of the de Sitter point demands that

$$(1 + x_1^2)^{n+2} \geq 1 + (n+2)x_1^2 + (n+1)(2n+1)x_1^4, \quad (11.35)$$

with

$$\lambda = \frac{x_d(1 + x_1^2)^{n+1}}{2[(1 + x_1^2)^{n+1} - 1 - (n+1)x_1^2]}. \quad (11.36)$$

For given n , a lower bound on λ follows from the condition (11.35).

For the model (iii), the Ricci scalar R_1 at the de Sitter point obeys

$$\lambda = \frac{x_1 \cosh^2(x_1)}{2 \sinh(x_1) \cosh(x_1) - x_1}, \quad (11.37)$$

where $x_1 = R_1/R_0$. The stability condition (11.32) gives the bounds

$$\lambda > 0.905, \quad x_1 > 0.920. \quad (11.38)$$

In what follows, we discuss the evolution of the dark energy equation of state for cosmologically viable $f(R)$ models explained above. For the confrontation of models with SN Ia observations, we rewrite the background equations (11.18) and (11.19) in the forms analogous to those in GR as [17, 25]

$$3M_{\text{pl}}^2 H^2 = \rho_m + \rho_{\text{DE}}, \quad (11.39)$$

$$-2M_{\text{pl}}^2 \dot{H} = \rho_m + \rho_{\text{DE}} + P_{\text{DE}}, \quad (11.40)$$

where

$$\rho_{\text{DE}} \equiv M_{\text{pl}}^2 \left[\frac{1}{2}(f_{,R}R - f) - 3H\dot{f}_{,R} + 3H^2(1 - f_{,R}) \right], \quad (11.41)$$

$$P_{\text{DE}} \equiv M_{\text{pl}}^2 \left[\ddot{f}_{,R} + 2H\dot{f}_{,R} - \frac{1}{2}(f_{,R}R - f) - (3H^2 + 2\dot{H})(1 - f_{,R}) \right]. \quad (11.42)$$

Defining ρ_{DE} and P_{DE} in this way, the standard continuity equation

$$\dot{\rho}_{\text{DE}} + 3H(\rho_{\text{DE}} + P_{\text{DE}}) = 0 \quad (11.43)$$

holds for the dark sector (see also Refs. [26, 27]) for related works).

The dark energy equation of state to be confronted with SN Ia observations can be defined by $w_{\text{DE}} \equiv P_{\text{DE}}/\rho_{\text{DE}}$. From Eqs. (11.41) and (11.42), it is given by

$$w_{\text{DE}} = -\frac{f_{,R}R - f + 2(3H^2 + 2\dot{H})(1 - f_{,R}) - 2\ddot{f}_{,R} - 4H\dot{f}_{,R}}{f_{,R}R - f + 6H^2(1 - f_{,R}) - 6H\dot{f}_{,R}}. \quad (11.44)$$

In viable $f(R)$ models (11.14)–(11.16), the quantity $f_{,R}$ approaches 1 in the asymptotic past ($R \gg R_0$), so w_{DE} starts to evolve from the value close to -1 . In this regime the scalar degree of freedom is nearly frozen. This reflects the fact that the mass squared (11.12) goes to infinity in the limit $R \rightarrow \infty$. In the asymptotic future the solutions approach the de Sitter fixed point characterized by constant H and $f_{,R}$, at which $w_{\text{DE}} = -1$. In the intermediate regime the dark energy equation of state deviates from -1 due to the time variation of $f_{,R}$.

In Fig. 11.1, we plot the evolution of w_{DE} versus the redshift z for the model (ii) with several different values of n and λ . The dark energy equation of state, which is initially close to -1 , decreases toward a minimum value smaller than -1 . Then it starts to increase and crosses the cosmological constant boundary. Finally, it approaches the asymptotic value $w_{\text{DE}} = -1$ with oscillations. Thus the $f(R)$ dark energy model (ii) gives rise to a phantom equation of state without violating stability conditions (11.11) and (11.13). The deviation of w_{DE} from -1 tends to be

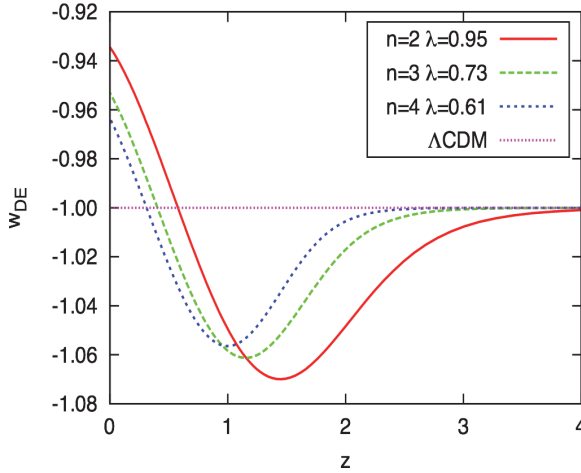


Fig. 11.1. The dark energy equation of state w_{DE} versus the redshift z for the $f(R)$ model (ii) with several different combinations of n and λ . The phantom equation of state ($w_{\text{DE}} < -1$) and the cosmological constant boundary crossing can be realized before reaching the de Sitter attractor. Reproduced from Ref. [25].

smaller for larger values of n . In fact, the Λ CDM model corresponds to the limit $n \rightarrow \infty$. Provided that $n \gtrsim \mathcal{O}(1)$ with λ of the order of unity, the $f(R)$ models (i) and (ii) are consistent with the joint observational constraints of SN Ia, CMB, and BAO [28–30].

In $f(R)$ gravity, the growth rate of matter density perturbations is larger than that in GR, so this leaves observational signatures in the measurement of large-scale structures and weak lensing. In Sec. 12.4.1, we will study the evolution of cosmological perturbations in $f(R)$ dark energy models to place further constraints on the allowed parameter space.

11.2. Brans–Dicke theories

The metric $f(R)$ gravity discussed in Sec. 11.1 belongs to a class of more general theories dubbed Brans–Dicke (BD) theories [31]. In BD theories, the Ricci scalar R is coupled to a scalar field χ with the coupling of the form χR . Taking into account a scalar potential $V(\chi)$ and matter fields, the action of BD theories is given by

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} \chi R - \frac{M_{\text{pl}}^2 \omega_{\text{BD}}}{2\chi} (\nabla\chi)^2 - V(\chi) \right] + \int d^4x L_m(g_{\mu\nu}, \Psi_m), \quad (11.45)$$

where $(\nabla\chi)^2 \equiv g^{\mu\nu} \nabla_\mu \chi \nabla_\nu \chi$ is the kinetic energy of the dimensionless scalar field χ , ω_{BD} is a constant called the BD parameter, L_m is the matter Lagrangian that depends on the metric $g_{\mu\nu}$ and matter fields Ψ_m . The original BD theory [31] corresponds to $V(\chi) = 0$, i.e., a massless scalar field. We require the condition $\chi > 0$ to avoid repulsive gravity.

We assume that matter fields are minimally coupled to gravity in the so-called Jordan frame given by the action (11.45) [32]. In this frame, the matter energy–momentum tensor $T_{\mu\nu}^{(m)} = -(2/\sqrt{-g})\delta L_m/\delta g^{\mu\nu}$ obeys the continuity equation

$$\nabla^\mu T_{\mu\nu}^{(m)} = 0. \quad (11.46)$$

The gravitational equations of motion can be derived by following the similar procedure to that explained in $f(R)$ gravity in Sec. 11.1. On using Eqs. (3.95) and (11.5), the variation of the action (11.45) with respect to $g^{\mu\nu}$ leads to

$$\delta S = \frac{M_{\text{pl}}^2}{2} \int d^4x \sqrt{-g} \left(\mathcal{G}_{\mu\nu} - \frac{T_{\mu\nu}}{M_{\text{pl}}^2} \right) \delta g^{\mu\nu}, \quad (11.47)$$

where

$$\mathcal{G}_{\mu\nu} \equiv \chi G_{\mu\nu} - \frac{\omega_{\text{BD}}}{\chi} \nabla_\mu \chi \nabla_\nu \chi + \left[\frac{\omega_{\text{BD}}}{2\chi} (\nabla\chi)^2 + \frac{V}{M_{\text{pl}}^2} \right] g_{\mu\nu} - \nabla_\mu \nabla_\nu \chi + g_{\mu\nu} \square \chi. \quad (11.48)$$

Hence the gravitational equations in BD theories are given by

$$M_{\text{pl}}^2 \mathcal{G}_{\mu\nu} = T_{\mu\nu}. \quad (11.49)$$

Variation of the action (11.45) with respect to χ leads to the Euler–Lagrange equation

$$\frac{\partial(\sqrt{-g}\mathcal{L})}{\partial\chi} - \nabla_\mu \left(\frac{\partial(\sqrt{-g}\mathcal{L})}{\partial(\nabla_\mu\chi)} \right) = 0, \quad (11.50)$$

where $\mathcal{L}$ is the Lagrangian density in the square bracket of Eq. (11.45). This gives rise to the scalar-field equation

$$\omega_{\text{BD}}\Box\chi - \frac{\omega_{\text{BD}}}{2\chi}(\nabla\chi)^2 - \frac{\chi V_{,\chi}}{M_{\text{pl}}^2} + \frac{1}{2}\chi R = 0. \quad (11.51)$$

In the Jordan frame, the field χ has a direct coupling to R . Since the matter sector is coupled to gravity, there is an extra force (fifth force) between the field χ and matter. If we transform the action (11.45) to the one in which the scalar field does not have a direct coupling with the Ricci scalar, the coupling between the scalar field and the matter sector becomes transparent. This new frame is called an Einstein frame, which we will discuss in the next section.

11.2.1. *Einstein frame and the scalar–matter coupling*

To transform the action (11.45) to that in the Einstein frame, we perform the conformal transformation [32]

$$\hat{g}_{\mu\nu} = \Omega^2(x)g_{\mu\nu}. \quad (11.52)$$

In Eq. (11.52), the conformal factor Ω is a function of spacetime point x . The line element $ds^2 = g_{\mu\nu}dx^\mu dx^\nu$ is transformed to $\hat{ds}^2 = \Omega^2(x)ds^2$ under the conformal transformation. In the following, the quantities with an over-hat represent those in the Einstein frame.

From Eq. (11.52), the metric tensor with an upper index and the determinant of the metric transform, respectively, as

$$g^{\mu\nu} = \Omega^2 \hat{g}^{\mu\nu}, \quad \sqrt{-g} = \Omega^{-4} \sqrt{-\hat{g}}. \quad (11.53)$$

The transformation of the Ricci scalar is given by [33]

$$R = \Omega^2 \left[\hat{R} + 6\hat{\Box}\omega - 6(\hat{\nabla}\omega)^2 \right], \quad (11.54)$$

where $\omega = \ln \Omega$, $\hat{\Box}\omega = \partial_\mu(\sqrt{-\hat{g}}\hat{g}^{\mu\nu}\partial_\nu\omega)/\sqrt{-\hat{g}}$, and $(\hat{\nabla}\omega)^2 = \hat{g}^{\mu\nu}\partial_\mu\omega\partial_\nu\omega$, with $\partial_\mu\omega = \partial\omega/\partial\hat{x}^\mu$. Substituting Eqs. (11.53) and (11.54) into Eq. (11.45), it follows

that the field χ does not have a direct coupling with $\hat{R}$ for the choice

$$\Omega = \sqrt{\chi}. \quad (11.55)$$

In this case, we have that $2\omega = \ln \chi$ and $(\nabla\chi)^2 = \chi(\hat{\nabla}\chi)^2$. Then, the resulting action in the Einstein frame reads

$$S_E = \int d^4x \sqrt{-\hat{g}} \left[\frac{1}{2} M_{\text{pl}}^2 \hat{R} - M_{\text{pl}}^2 (3 + 2\omega_{\text{BD}}) (\hat{\nabla}\omega)^2 - \frac{V(\chi)}{\chi^2} \right] \\ + \int d^4x L_m(\Omega^{-2} \hat{g}_{\mu\nu}, \Psi_m), \quad (11.56)$$

where we have dropped the boundary term $\hat{\square}\omega$ irrelevant to the dynamics.

If $\omega_{\text{BD}} < -3/2$, then the kinetic term in Eq. (11.56) has a wrong sign, so it corresponds to a ghost state. In the following, we shall focus on the case

$$\omega_{\text{BD}} > -\frac{3}{2}, \quad (11.57)$$

under which the ghost is absent. Introducing a canonical scalar field ϕ , as

$$\phi = M_{\text{pl}} \sqrt{(3 + 2\omega_{\text{BD}})/2} \ln \chi, \quad (11.58)$$

the action (11.56) can be written in the form

$$S_E = \int d^4x \sqrt{-\hat{g}} \left[\frac{1}{2} M_{\text{pl}}^2 \hat{R} - \frac{1}{2} (\hat{\nabla}\phi)^2 - \hat{V}(\phi) \right] \\ + \int d^4x L_m(\chi^{-1} \hat{g}_{\mu\nu}, \Psi_m), \quad (11.59)$$

where

$$\hat{V}(\phi) \equiv \frac{V(\chi(\phi))}{\chi^2}. \quad (11.60)$$

In the Einstein-frame action (11.59), the scalar field χ is coupled to matter through the metric $\hat{g}_{\mu\nu}$. To quantify the interaction between the scalar field and matter, we introduce the coupling constant Q in the form

$$\chi = e^{-2Q\phi/M_{\text{pl}}}. \quad (11.61)$$

On using Eq. (11.58), we obtain the relation

$$3 + 2\omega_{\text{BD}} = \frac{1}{2Q^2}, \quad (11.62)$$

which is valid under the no-ghost condition (11.57). Then, the Jordan-frame action (11.45) can be expressed as

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} e^{-2Q\phi/M_{\text{pl}}} R - \frac{1}{2} (1 - 6Q^2) e^{-2Q\phi/M_{\text{pl}}} (\nabla\phi)^2 - V(\phi) \right] + \int d^4x L_m(g_{\mu\nu}, \Psi_m). \quad (11.63)$$

In the limit that $Q \rightarrow 0$, the action (11.63) reduces to that of the minimally coupled scalar field in GR (quintessence). From Eq. (11.62), this limit corresponds to $\omega_{\text{BD}} \rightarrow \infty$. For larger $|Q|$, the interaction between the scalar field and matter appearing in the matter Lagrangian L_m of Eq. (11.59) is stronger.

Let us derive the equation of the scalar field ϕ in the Einstein frame. Varying the action (11.59) with respect to ϕ , it follows that

$$\hat{\square}\phi - \hat{V}_{,\phi} + \frac{1}{\sqrt{-\hat{g}}} \frac{\partial L_m}{\partial \phi} = 0. \quad (11.64)$$

On using the relations (11.53) with $\Omega^2 = \chi$, the matter energy-momentum tensor $\hat{T}_{\mu\nu}^{(m)}$ in the Einstein frame is related to that in the Jordan frame, as

$$\hat{T}_{\mu\nu}^{(m)} = -\frac{2}{\sqrt{-\hat{g}}} \frac{\delta L_m}{\delta \hat{g}^{\mu\nu}} = \frac{T_{\mu\nu}^{(m)}}{\chi}. \quad (11.65)$$

Now, we consider a perfect fluid whose energy-momentum tensor in the Einstein frame is given by

$$\tilde{T}_{\nu}^{\mu(m)} = \text{diag}(-\hat{\rho}_m, \hat{P}_m, \hat{P}_m, \hat{P}_m) = \text{diag}\left(-\frac{\rho_m}{\chi^2}, \frac{P_m}{\chi^2}, \frac{P_m}{\chi^2}, \frac{P_m}{\chi^2}\right), \quad (11.66)$$

where ρ_m and P_m are the energy density and the pressure in the Jordan frame, respectively. The derivative of the Lagrangian density $L_m = L_m(g_{\mu\nu}, \Psi_m) = L_m(\chi^{-1}(\phi)\hat{g}_{\mu\nu}, \Psi_m)$ with respect to ϕ is

$$\begin{aligned} \frac{\partial L_m}{\partial \phi} &= \frac{\delta L_m}{\delta g^{\mu\nu}} \frac{\partial g^{\mu\nu}}{\partial \phi} \\ &= \frac{1}{\chi(\phi)} \frac{\delta L_m}{\delta \hat{g}^{\mu\nu}} \frac{\partial(\chi(\phi)\hat{g}^{\mu\nu})}{\partial \phi} = \sqrt{-\hat{g}} \frac{Q}{M_{\text{pl}}} \hat{g}^{\mu\nu} \hat{T}_{\mu\nu}^{(m)} = \sqrt{-\hat{g}} \frac{Q}{M_{\text{pl}}} \hat{T}_m, \end{aligned} \quad (11.67)$$

where $\hat{T}_m = \hat{g}^{\mu\nu} \hat{T}_{\mu\nu}^{(m)}$ is the trace of matter in the Einstein frame. Then, Eq. (11.64) reduces to

$$\hat{\square}\phi - \hat{V}_{,\phi} + \frac{Q}{M_{\text{pl}}} \hat{T}_m = 0. \quad (11.68)$$

For perfect fluids we have that $\hat{T}_m = -\hat{\rho}_m + 3\hat{P}_m$, so the last term on the left hand side of Eq. (11.68) does not vanish except for the radiation ($\hat{\rho}_m = 3\hat{P}_m$). This means

that, in the Einstein frame, the scalar field has an explicit coupling with the matter sector.

For concreteness, let us consider the flat FLRW background given by the line element in the Einstein frame

$$d\hat{s}^2 = -d\hat{t}^2 + \hat{a}^2(\hat{t})d\mathbf{x}^2. \quad (11.69)$$

In this case, the field equation (11.68) reads

$$\frac{d^2\phi}{d\hat{t}^2} + 3\hat{H}\frac{d\phi}{d\hat{t}} + \hat{V}_{,\phi} = -\frac{Q}{M_{\text{pl}}} \left(\hat{\rho}_m - 3\hat{P}_m \right), \quad (11.70)$$

where $\hat{H} = (d\hat{a}/d\hat{t})/\hat{a}$ is the Hubble parameter in the Einstein frame. In terms of the field density $\hat{\rho}_\phi = (d\phi/d\hat{t})^2/2 + \hat{V}(\phi)$ and the pressure $\hat{P}_\phi = (d\phi/d\hat{t})^2/2 - \hat{V}(\phi)$, we can write Eq. (11.70) in the form

$$\frac{d\hat{\rho}_\phi}{d\hat{t}} + 3\hat{H} \left(\hat{\rho}_\phi + \hat{P}_\phi \right) = -\frac{Q}{M_{\text{pl}}} \left(\hat{\rho}_m - 3\hat{P}_m \right) \frac{d\phi}{d\hat{t}}. \quad (11.71)$$

The matter sector obeys the continuity equation (11.46) in the Jordan frame, which reduces to $\dot{\rho}_m + 3H(\rho_m + P_m) = 0$ on the flat FLRW background. Since the line element $ds^2 = -dt^2 + a^2(t)d\mathbf{x}^2$ in the Jordan frame is related to that in the Einstein frame, as $d\hat{s}^2 = \Omega^2 ds^2 = \chi ds^2$, we obtain the relations

$$d\hat{t} = \sqrt{\chi} dt, \quad \hat{a} = \sqrt{\chi} a. \quad (11.72)$$

Then, the Hubble parameter in the Jordan frame has a relation with $\hat{H}$, as $H = F^{1/2}[\hat{H} - (d\chi/d\hat{t})/(2\chi)]$. On using the relations $\rho_m = \chi^2 \hat{\rho}_m$ and $P_m = \chi^2 \hat{P}_m$, the matter continuity equation can be expressed as

$$\frac{d\hat{\rho}_m}{d\hat{t}} + 3\hat{H} \left(\hat{\rho}_m + \hat{P}_m \right) = \frac{Q}{M_{\text{pl}}} \left(\hat{\rho}_m - 3\hat{P}_m \right) \frac{d\phi}{d\hat{t}}. \quad (11.73)$$

From Eqs. (11.71) and (11.73), it is clear that the scalar field ϕ and matter directly interacts with each other in the Einstein frame. Taking the non-relativistic limit $\hat{P}_m \rightarrow 0$, Eqs. (11.70) and (11.73) are equivalent to Eqs. (10.115) and (10.116), respectively, derived for coupled quintessence. Thus, after the conformal transformation to the Einstein frame, the interaction of the forms (10.110) and (10.111) with the coupling (10.112) arises in BD theories [34, 35].

The metric $f(R)$ gravity discussed in Sec. 11.1 belongs to a sub-class of BD theories. Let us consider the following action:

$$S = \frac{M_{\text{pl}}^2}{2} \int d^4x \sqrt{-g} [f(\varphi) + f_{,\varphi}(R - \varphi)] + \int d^4x L_m(g_{\mu\nu}, \Psi_m), \quad (11.74)$$

where φ is a scalar quantity. Variation of this action leads to

$$f_{,\varphi\varphi}(R - \varphi) = 0. \quad (11.75)$$

As long as $f_{,\varphi\varphi} \neq 0$, we have that $\varphi = R$. In this case, the action (11.74) is equivalent to the action (11.1) of $f(R)$ gravity. If we define

$$\chi \equiv f_{,\varphi}, \quad (11.76)$$

the action (11.74) can be expressed as

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} \chi R - V(\chi) \right] + \int d^4x L_m(g_{\mu\nu}, \Psi_m), \quad (11.77)$$

where

$$V(\chi) = \frac{M_{\text{pl}}^2}{2} [\chi \varphi(\chi) - f(\varphi(\chi))]. \quad (11.78)$$

Comparing the action (11.77) with Eq. (11.45), it follows that metric $f(R)$ gravity belongs to a special case of BD theories with the BD parameter [36, 37]

$$\omega_{\text{BD}} = 0. \quad (11.79)$$

The field χ corresponds to $f_{,R}$, which is a dynamical quantity in $f(R)$ gravity. From Eqs. (11.58) and (11.60), the scalar field ϕ and the potential $\hat{V}(\phi)$ in the Einstein frame are

$$\phi = \sqrt{\frac{3}{2}} M_{\text{pl}} \ln f_{,R}(R), \quad (11.80)$$

$$\hat{V}(\phi) = \frac{M_{\text{pl}}^2}{2} e^{-\frac{2\sqrt{6}}{3} \frac{\phi}{M_{\text{pl}}}} (f_{,RR} - f). \quad (11.81)$$

Provided that $f_{,R}(R)$ is not constant, the field ϕ behaves as a dynamical scalar degree of freedom with the potential $\hat{V}(\phi)$ of a gravitational origin. Comparing Eq. (11.61) with Eq. (11.80), the metric $f(R)$ gravity corresponds to the coupling

$$Q = -\frac{1}{\sqrt{6}}. \quad (11.82)$$

Hence the gravitational scalar field ϕ interacts with matter with the coupling $|Q| \simeq 0.4$ in the Einstein frame.

From the above discussion, the BD theories give rise to a universal coupling Q between the scalar field and matter (dark matter and baryons) in the Einstein frame. Especially, the coupling between the scalar field and baryons leads to the propagation of fifth forces. In the absence of the scalar potential $\hat{V}(\phi)$, the scalar field freely propagates to mediate fifth forces with baryons. For such a massless scalar field, gravitational experiments in the solar system constrained the BD parameter to be [38]

$$\omega_{\text{BD}} > 40000. \quad (11.83)$$

On using the relation (11.62), this bound translates

$$|Q| < 2.5 \times 10^{-3}. \quad (11.84)$$

The bound (11.84) cannot be applied to a massive scalar field with a potential $\hat{V}(\phi)$, e.g., $f(R)$ gravity. If the field is sufficiently massive in regions of high density, it is possible to suppress the propagation of fifth forces even for $|Q| = O(1)$ under the chameleon mechanism [34, 39]. For example, the $f(R)$ models (11.14)–(11.16) are designed to have a large field mass in the regime $R \gg R_0$. The models (11.14) and (11.15) can be consistent with solar-system constraints for $n \gtrsim 1$ [16, 40]. In Sec. 14.1, we will discuss the detail of the chameleon mechanism and apply it to dark energy models in the framework of $f(R)$ gravity and BD theories.

11.2.2. Background cosmological dynamics in BD theories

We have shown that BD theories have a coupling between the scalar field ϕ and matter in the Einstein frame. While we are dealing with the same physics in both Jordan and Einstein frames, using the different time and length scales leads to apparent difference between observables in two frames [41, 42]. When we confront BD theories with observations and experiments, we compute observables in the Jordan frame in which baryons obey the standard continuity equation ($\rho_m \propto a^{-3}$).

In the coupled dark energy scenario discussed in Sec. 10.3.1, the starting point was interacting energy–momentum tensors between the scalar field ϕ and dark matter given by Eqs. (10.110) and (10.111). It was assumed that baryons are decoupled to the scalar field. This is different from BD theories in the Einstein frame in which all non-relativistic matter species have a universal coupling Q with the scalar field ϕ . We are now interested in BD theories with the coupling in the range

$$10^{-3} \ll |Q| \lesssim 1, \quad (11.85)$$

which includes the case of metric $f(R)$ gravity. For a massless scalar field, the models with the coupling (11.85) are inconsistent with the local gravity bound (11.84), but this situation is different for a massive field with a potential $V(\phi)$. If the field is sufficiently massive in regions of high density, the chameleon mechanism allows a possibility for realizing an effective coupling Q_{eff} much smaller than the bare coupling Q .

For the construction of viable dark energy models in BD theories, we first discuss the Jordan-frame potential in $f(R)$ gravity ($Q = -1/\sqrt{6}$) and extend it to the case of general couplings. Let us consider the dark energy models (11.14) and (11.15) in $f(R)$ gravity. In the high-curvature regime characterized by $R \gg R_0$, these models have the asymptotic form (11.17). In the early Universe the cosmological evolution

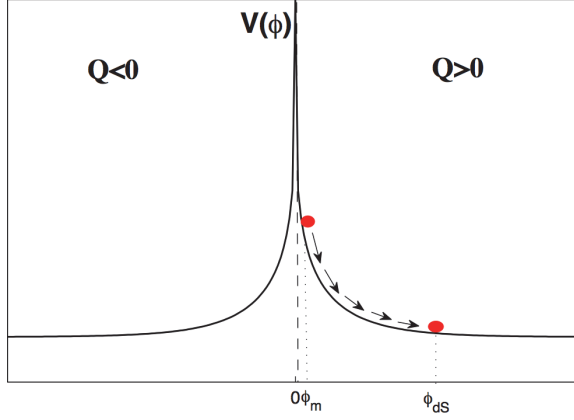


Fig. 11.2. The shape of the potential (11.88). For $Q > 0$ and $Q < 0$ the valid regions correspond to $\phi > 0$ and $\phi < 0$, respectively. The scalar field evolves along the instantaneous minima given by the condition $V_{,\phi} + M_{\text{pl}} Q F R = 0$. Reproduced from Ref. [35].

is similar to that in GR, but the deviation from GR arises after R decreases to the order of R_0 . On using Eq. (11.17), the scalar field ϕ defined by Eq. (11.80) reads

$$\phi \simeq \sqrt{\frac{3}{2}} M_{\text{pl}} \ln \left[1 - 2n\lambda \left(\frac{R}{R_0} \right)^{-(2n+1)} \right] < 0, \quad (11.86)$$

which approaches 0 in the limit $R \rightarrow \infty$. The potential (11.78) in the Jordan frame is given by

$$V(\phi) \simeq \frac{\lambda R_0 M_{\text{pl}}^2}{2} \left[1 - \frac{2n+1}{(2n\lambda)^{2n/(2n+1)}} \left(1 - e^{\sqrt{2/3}\phi/M_{\text{pl}}} \right)^{2n/(2n+1)} \right], \quad (11.87)$$

which approaches the constant $\lambda R_0 M_{\text{pl}}^2/2$ for $R \rightarrow \infty$. For increasing R , the mass squared $m_\phi^2 = V_{,\phi\phi}$ gets larger. In the limit that $R \rightarrow \infty$, we have $m_\phi^2 \rightarrow \infty$ (see Fig. 11.2 for $Q < 0$). After R decreases to the order of R_0 , the mass squared approaches the order of $R_0 \sim H_0^2$ for n and λ of the order of 1.

The $f(R)$ gravity corresponds to $Q = -1/\sqrt{6}$, but it is possible to extend the above discussion to the case of general couplings Q . For example, let us consider the extended version of the potential (11.87) [35]

$$V(\phi) = V_0 \left[1 - C(1 - e^{-2Q\phi/M_{\text{pl}}})^p \right] \quad (V_0 > 0, 0 < C < 1, 0 < p < 1). \quad (11.88)$$

This potential is defined in the region $\phi > 0$ for $Q > 0$ and in the region $\phi < 0$ for $Q < 0$, see Fig. 11.2 for the illustration. We assume that the coupling $|Q|$ is at least of the order of 0.1.

For concreteness, we discuss the cosmology in BD theories given by the action (11.63) in the Jordan frame. As a matter action S_m , we consider a perfect fluid of non-relativistic matter with the energy density ρ_m . On the flat FLRW background the equations of motion are given by

$$3M_{\text{pl}}^2 F H^2 = \frac{1}{2}(1 - 6Q^2)F\dot{\phi}^2 + V - 3M_{\text{pl}}^2 H\dot{F} + \rho_m, \quad (11.89)$$

$$2M_{\text{pl}}^2 F\dot{H} = -(1 - 6Q^2)F\dot{\phi}^2 - M_{\text{pl}}^2 \ddot{F} + M_{\text{pl}}^2 H\dot{F} - \rho_m, \quad (11.90)$$

where $F = e^{-2Q\phi/M_{\text{pl}}}$, and the continuity equation $\dot{\rho}_m + 3H\rho_m = 0$ holds for non-relativistic matter. Varying the action (11.63) with respect to ϕ , it follows that

$$(1 - 6Q^2)F \left(\ddot{\phi} + 3H\dot{\phi} + \frac{\dot{F}}{2F}\dot{\phi} \right) + V_{,\phi} + M_{\text{pl}}QFR = 0. \quad (11.91)$$

From Eqs. (11.89) and (11.90), the Ricci scalar $R = 6(2H^2 + \dot{H})$ is

$$R = -(1 - 6Q^2)\frac{\dot{\phi}^2}{M_{\text{pl}}^2} + \frac{4V}{M_{\text{pl}}^2 F} - \frac{3}{F}(\ddot{F} + 3H\dot{F}) + \frac{\rho_m}{M_{\text{pl}}^2 F}. \quad (11.92)$$

Since $R \simeq \rho_m/(M_{\text{pl}}^2 F)$ during the matter-dominated epoch, there exist instantaneous minima at $\phi = \phi_m$ satisfying

$$V_{,\phi}(\phi_m) + \frac{Q\rho_m}{M_{\text{pl}}} = 0, \quad (11.93)$$

where ϕ_m changes with the decrease of ρ_m [35]. For the potential (11.88), we have

$$\phi_m \simeq \frac{M_{\text{pl}}}{2Q} \left(\frac{2V_0 p C}{\rho_m} \right)^{1/(1-p)}. \quad (11.94)$$

The field ϕ evolves slowly along the instantaneous minima. As in the case of $f(R)$ gravity, the field value ϕ_m approaches 0 in the asymptotic past ($\rho_m \gg V_0 p C$). With the decrease of ρ_m , $|\phi_m|$ deviates from 0.

For the potential (11.88), the quantity $\lambda(\phi) = -M_{\text{pl}}V_{,\phi}/V$ is given by

$$\lambda(\phi) = \frac{2CpQe^{-2Q\phi/M_{\text{pl}}}(1 - e^{-2Q\phi/M_{\text{pl}}})^{p-1}}{1 - C(1 - e^{-2Q\phi/M_{\text{pl}}})^p}. \quad (11.95)$$

In the limit that $\phi \rightarrow 0$, we have $|\lambda(\phi)| \rightarrow \infty$ and $V(\phi) \rightarrow V_0$. As the field $|\phi|$ increases in time, the parameter $|\lambda(\phi)|$ decreases. In the limit that $|\phi| \rightarrow \infty$, the potential $V(\phi)$ approaches the constant $V_0(1 - C)$. In the early cosmological epoch, the model is close to the Λ CDM model with the potential energy V_0 much smaller than ρ_m .

At late times, the deviation from the Λ CDM model arises with the decrease of $|\lambda(\phi)|$. After the Universe enters the epoch of cosmic acceleration, the potential energy V dominates over ρ_m and hence $R \simeq 4V/(M_{\text{pl}}^2 F)$ from Eq. (11.92). From Eq. (11.91), there is a minimum at $\phi = \phi_{\text{dS}}$ obeying the condition

$$V_{,\phi}(\phi_{\text{dS}}) + \frac{4Q}{M_{\text{pl}}} V(\phi_{\text{dS}}) = 0, \quad (11.96)$$

which corresponds to $\lambda(\phi_{\text{dS}}) = 4Q$. This is a de Sitter solution satisfying $\dot{\phi} = 0$ and $V = 3M_{\text{pl}}^2 F H^2 = \text{constant}$. In $f(R)$ gravity, the condition (11.96) translates to $RF = 2f$ with $F = f_{,R}$ by using Eqs. (11.78), (11.80), and (11.81). This agrees with the condition (11.9) for the existence of de Sitter solutions in $f(R)$ gravity. For the potential (11.88), the field value at the de Sitter fixed point obeys

$$C(1 - F_{\text{dS}})^{p-1}[2 + (p-2)F_{\text{dS}}] = 2, \quad (11.97)$$

where $F_{\text{dS}} \equiv F(\phi_{\text{dS}})$. The stability of the de Sitter point is known by perturbing the background equations of motion around $\phi = \phi_{\text{dS}}$ and $H = H_{\text{dS}}$. Since the corresponding eigenvalues of the Jacobian matrix at $\phi = \phi_{\text{dS}}$ are given by $\mu_{\pm} = -(3/2)[1 \pm \sqrt{1 + (4M_{\text{pl}}/3)d\lambda/d\phi}]$, the de Sitter point is stable for

$$\frac{d\lambda}{d\phi}(\phi_{\text{dS}}) < 0. \quad (11.98)$$

For the potential (11.88), the condition (11.98) is satisfied for $1 - pF_{\text{dS}} > C(1 - F_{\text{dS}})^p$. On using Eq. (11.88), this condition translates to

$$F_{\text{dS}} > \frac{1}{2-p}. \quad (11.99)$$

Note that, for $0 < C < 1$, the stability condition of the de Sitter point is always satisfied.

The background cosmological dynamics is different from that of the coupled quintessence scenario studied in Sec. 10.3.1, in that the analysis in the present section is carried out in the Jordan frame with $\lambda(\phi)$ changing in time. The ϕ MDE fixed point derived in the Einstein frame in Sec. 10.3.1 also exists in the Jordan frame, but for the large coupling we are discussing now ($|Q| \gtrsim 0.1$), the corresponding ϕ MDE in the Jordan frame is not cosmologically acceptable. Instead, the field is nearly frozen around $\phi = \phi_m$ during the early matter era with the small energy density of the order of $V_0 \approx M_{\text{pl}}^2 H_0^2 \ll \rho_m$. As $|\lambda(\phi)|$ decreases, the variation of the field tends to be important at a later cosmological epoch. The solutions finally approach the de Sitter fixed point satisfying $\lambda(\phi_{\text{dS}}) = 4Q$.

We can write Eqs. (11.89) and (11.90) in the forms (11.39) and (11.40), respectively, by defining

$$\rho_{\text{DE}} = \frac{1}{2}(1 - 6Q^2)F\dot{\phi}^2 + V + 3M_{\text{pl}}^2 H^2(1 - F) - 3M_{\text{pl}}^2 H\dot{F}, \quad (11.100)$$

$$P_{\text{DE}} = \frac{1}{2}(1 - 6Q^2)F\dot{\phi}^2 - V - M_{\text{pl}}^2(3H^2 + 2\dot{H})(1 - F) + M_{\text{pl}}^2(\ddot{F} + 2H\dot{F}). \quad (11.101)$$

Since the energy density ρ_{DE} and the pressure P_{DE} obey the usual continuity equation $\dot{\rho}_{\text{DE}} + 3H(\rho_{\text{DE}} + P_{\text{DE}}) = 0$, the resulting dark energy equation of state is given by $w_{\text{DE}} = P_{\text{DE}}/\rho_{\text{DE}}$. In the regime $R \gg R_0$, we have $F \rightarrow 1$, $\dot{\phi}^2 \rightarrow 0$, and $V \rightarrow V_0$, so that $\rho_{\text{DE}} \simeq -P_{\text{DE}} \simeq V_0$ and $w_{\text{DE}} \rightarrow -1$. At the de Sitter fixed point, we have $\rho_{\text{DE}} \simeq -P_{\text{DE}} \simeq V + 3M_{\text{pl}}^2 H^2(1 - F)$ and hence $w_{\text{DE}} \rightarrow -1$. When the field ϕ evolves from the instantaneous minima ϕ_m to the de Sitter value ϕ_{dS} , the field velocity $\dot{\phi}$ also contributes to ρ_{DE} and P_{DE} . During this transition, w_{DE} enters the phantom region ($w_{\text{DE}} < -1$) and finally approaches the value -1 at the de Sitter fixed point. The evolution of w_{DE} is similar to that plotted in Fig. 11.1 in the context of $f(R)$ gravity, so the dark energy models in BD theories with large couplings $|Q|$ ($\gtrsim 0.1$) can be distinguished from modified matter models like quintessence and k-essence (in which $w_{\text{DE}} \geq -1$).

11.3. Galileons

There is another class of modified gravity models of dark energy based on braneworlds. In braneworlds, standard model particles are confined on a three-dimensional brane embedded in a five-dimensional bulk spacetime with large extra dimensions [43]. In the so-called Dvali-Gabadadze-Porrati (DGP) model [44], the three-brane is embedded in a Minkowski bulk spacetime with an infinitely large extra dimension. The DGP model allows the existence of a self-accelerating solution on the three-brane due to a gravitational leakage to the extra dimension. However, the self-accelerating solution is plagued by the ghost problem [45–47], in addition to the incompatibility with the observational data of SN Ia, BAO, and CMB [48, 49].

In the DGP model, there exists another healthy branch of solutions without ghosts. Although this does not allow self-accelerating solutions, the effective action on the brane after integrating out the bulk contribution provides a rich phenomenology. In the decoupling limit of the DGP model, the effective action reduces to a theory of a scalar field ϕ with a cubic self-interaction $(\nabla_\mu \phi \nabla^\mu \phi) \square \phi$, where ϕ represents the brane position in the extra dimension. The field equation of motion following from this self-interaction is invariant under the Galilean transformation

$$\phi \rightarrow \phi + b_\mu x^\mu + c, \quad (11.102)$$

where b_μ and c are constants. The cubic interaction mentioned above is not the only term respecting the Galilean symmetry, but there are also other field derivatives invariant under the Galilean shift [50, 51]. The scalar field with derivative interactions respecting the Galilean symmetry is called the Galileon [51].

In the Minkowski spacetime, the Galileon obeys second-order differential equations of motion. This second-order property allows us to avoid the so-called Ostrogradski instability associated with the Hamiltonian unbounded from below [52]. In the curved spacetime, the simple replacement of partial derivatives with covariant derivatives in the Galileon Lagrangian gives rise to the equations of motion higher than second order. Deffayet *et al.* [53, 54] derived full Lagrangians of the covariant Galileon with second-order equations of motion on general curved backgrounds. This can be achieved by introducing field-derivative couplings with the Ricci scalar R and the Einstein tensor $G_{\nu\rho}$. In the Minkowski limit, the covariant Galileon Lagrangian recovers that derived in Ref. [51]. In the DGP decoupling theory with a relativistic probe brane embedded in the five-dimensional bulk, all the derivative self-interactions of covariant Galileons follow from the brane tension, induced curvature, and Gibbons–Hawking–York boundary terms [55].

The covariant Galileon allows the existence of de Sitter solutions relevant to the late-time cosmic acceleration [56–58] (see also Refs. [59, 60] for the application to inflation). Moreover, there exists a tracker solution during the radiation and matter eras. Unlike the DGP model, it is also possible to find parameter spaces in which ghosts and Laplacian instabilities of scalar and tensor perturbations are absent [57, 58].

In what follows, we will first discuss the problem associated with theories containing derivatives higher than second order (i.e., the Ostrogradski instability) and then proceed to the construction of second-order Galileon Lagrangians in Minkowski spacetime. Then, we generalize the Minkowski Galileon to that in curved spacetime. We also study the background cosmology in the presence of covariant Galileons and matter perfect fluids. The evolution of cosmological perturbations and the screening mechanism of fifth forces will be discussed in Secs. 12.4.3 and 14.2.3, respectively.

11.3.1. Ostrogradski instability

The Ostrogradski instability corresponds to a linear instability of the Hamiltonian arising for theories containing derivatives higher than second order in their equations of motion [52, 61, 62]. For simplicity, we consider the one-dimensional motion of a point particle whose position depends on the time t , as $q(t)$. In the analytical mechanics, the Lagrangian L depends on the position $q(t)$ and the velocity $\dot{q}(t)$. Now, we discuss the case in which the Lagrangian depends on time derivatives of q up to N th order. Then, the action on the Minkowski background is given by

$$S = \int L(q, \dot{q}, \ddot{q}, \dots, q^{(N)}) dt, \quad (11.103)$$

where $q^{(i)} \equiv d^i q / dt^i$. Variation of this action leads to

$$\delta S = \int \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} + \frac{\partial L}{\partial \ddot{q}} \delta \ddot{q} + \cdots + \frac{\partial L}{\partial q^{(N)}} \delta q^{(N)} \right) dt. \quad (11.104)$$

After integrations by parts, the action (11.104) reduces to

$$\delta S = \int \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) + \frac{d^2}{dt^2} \left(\frac{\partial L}{\partial \ddot{q}} \right) - \cdots + \left(-\frac{d}{dt} \right)^N \frac{\partial L}{\partial q^{(N)}} \right] \delta q dt. \quad (11.105)$$

From the variational principle $\delta S = 0$, we obtain the equation of motion

$$\sum_{i=0}^N \left(-\frac{d}{dt} \right)^i \frac{\partial L}{\partial q^{(i)}} = 0, \quad (11.106)$$

which contains the time derivatives up to $q^{(2N)}$. For $N = 1$, the Euler–Lagrange equation (11.106) remains of second order.

If the highest partial derivative $\partial L / \partial q^{(N)}$ depends on $q^{(N)}$, this is called non-degenerate [61]. In this case, the $2N$ th order derivative $q^{(2N)}$ can be solved in the form

$$q^{(2N)} = F \left(q, \dot{q}, \ddot{q}, \dots, q^{(2N-1)} \right). \quad (11.107)$$

The standard Newtonian mechanics corresponds to $N = 1$, in which case the second derivative $\ddot{q}$ depends on q and $\dot{q}$, as $\ddot{q} = F(q, \dot{q})$. Hence we only need to know the initial conditions of q and $\dot{q}$ at a given time t_0 to solve the dynamical equation of motion. For $N \geq 2$, we require the initial conditions of $q, \dot{q}, \ddot{q}, \dots, q^{(2N-1)}$ to close the system. In other words, the number of degrees of freedom increases for the theories containing time derivatives higher than first order in the Lagrangian.

Since the dynamics of the theory (11.103) depends on the $2N$ initial data, the system should be described by $2N$ canonical variables. The choices of Ostrogradski [52] are given by

$$Q_i \equiv q^{(i-1)}, \quad (11.108)$$

$$P_i \equiv \sum_{j=i}^N \left(-\frac{d}{dt} \right)^{j-i} \frac{\partial L}{\partial q^{(j)}}. \quad (11.109)$$

Now, we are considering the non-degenerate case in which the quantity $\partial L / \partial q^{(N)}$ depends on $q^{(N)}$. Since the Lagrangian L depends on $Q_1, Q_2, \dots, Q_N$ as well, we can solve the equation $\partial L / \partial q^{(N)} = P_N$ (which corresponds to Eq. (11.109) with $i = N$) to express $q^{(N)}$ in terms of $P_N, Q_1, Q_2, \dots, Q_N$, such that

$$q^{(N)} = f(P_N, Q_1, Q_2, \dots, Q_N). \quad (11.110)$$

The canonical Hamiltonian is given by

$$\begin{aligned}\mathcal{H} &\equiv \sum_{i=1}^N P_i q^{(i)} - L \\ &= \sum_{i=1}^{N-1} P_i Q_{i+1} + P_N f(P_N, Q_1, Q_2, \dots, Q_N) \\ &\quad - L(Q_1, Q_2, \dots, Q_N, f(P_N, Q_1, \dots, Q_N)).\end{aligned}\quad (11.111)$$

Then, the particle dynamics is governed by the canonical equations

$$\dot{Q}_i = \frac{\partial \mathcal{H}}{\partial P_i}, \quad (11.112)$$

$$\dot{P}_i = -\frac{\partial \mathcal{H}}{\partial Q_i}, \quad (11.113)$$

where $i = 1, 2, \dots, N$. From the $i = 1, 2, \dots, N - 1$ components of Eq. (11.112), we obtain the trivial relations $\dot{Q}_i = Q_{i+1}$. The partial derivative $\partial \mathcal{H} / \partial P_N$ is equivalent to $q^{(N)}$, i.e., $\dot{Q}_N$, so the $i = N$ component of Eq (11.112) is also satisfied. The $i = 1$ component of Eq. (11.113) reads

$$\dot{P}_1 = \frac{\partial L}{\partial q}. \quad (11.114)$$

From the definition of P_i given in Eq. (11.109), it follows that Eq. (11.114) corresponds to the Euler–Lagrange equation (11.106). The $i = 2, \dots, N$ components of Eq. (11.113) translate to

$$\dot{P}_i + P_{i-1} = \frac{\partial L}{\partial q^{(i-1)}}. \quad (11.115)$$

Taking the time derivative of Eq. (11.109) and adding the term P_{i-1} , we find that the left hand side of Eq. (11.115) is equivalent to $\partial L / \partial q^{(i-1)}$.

If the action (11.103) contains time derivatives of q up to first order, i.e., $S = \int L(q, \dot{q}) dt$, the canonical momentum yields $P = \partial L / \partial \dot{q}$. Under the non-degenerate condition, i.e., $\partial L / \partial \dot{q}$ depends on $\dot{q}$, we can express $\dot{q}$ in terms of p and q as $\dot{q} = f(P, q)$. Then, the canonical Hamiltonian $\mathcal{H} = P\dot{q} - L$ becomes $\mathcal{H} = Pf(P, q) - L(q, f(P, q))$. In this case the first term $Pf(P, q)$ is not generally linear in P . In Newton mechanics this term is associated with the kinetic energy proportional to P^2 , so it is bounded from below.

On the other hand, the Hamiltonian (11.111) contains the terms $P_1 Q_2, P_2 Q_3, \dots, P_{N-1} Q_N$, which are linear in $P_1, P_2, \dots, P_{N-1}$ respectively. This means that the Hamiltonian associated with the action (11.103) whose Lagrangian contains time derivatives higher than first order is not bounded from below. In other words, the unbounded negative energy can lead to a ghost-like instability of the system. This is called the Ostrogradski instability, which arises for the Lagrangian depending

non-degenerately upon $q^{(N)}$ with $N \geq 2$. The Ostrogradski instability is related to the appearance of extra degrees of freedom arising from time derivatives higher than second order in the dynamical equations of motion.

For example, we consider the Lagrangian of a harmonic oscillator in the presence of two derivative terms $\ddot{q}^2$ and $\beta\dot{q}^2\ddot{q}$ higher than first order, i.e.,

$$L = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2q^2 + \alpha\ddot{q}^2 + \beta\dot{q}^2\ddot{q}, \quad (11.116)$$

where m, ω, α, β are non-vanishing constants. The Euler–Lagrange equation (11.106), which is of fourth order, can be expressed as the non-degenerate form

$$q^{(4)} = \frac{1}{2\alpha} (m\ddot{q} + m\omega^2q). \quad (11.117)$$

The two canonical momenta (11.109) are given, respectively, by

$$P_1 = \frac{\partial L}{\partial \dot{q}} - \frac{d}{dt} \left(\frac{\partial L}{\partial \ddot{q}} \right) = m\dot{q} - 2\alpha\ddot{q}, \quad (11.118)$$

$$P_2 = \frac{\partial L}{\partial \ddot{q}} = 2\alpha\ddot{q} + \beta\dot{q}^2. \quad (11.119)$$

Then, the Hamiltonian (11.111) yields

$$\mathcal{H} = \frac{1}{2}m\dot{q}^2 + \frac{1}{2}m\omega^2q^2 + \alpha\ddot{q}^2 - 2\alpha\dot{q}\ddot{q}. \quad (11.120)$$

If $\alpha = 0$, then $\mathcal{H} = m\dot{q}^2/2 + m\omega^2q^2/2 \geq 0$. For $\alpha \neq 0$, the last term on the right hand side of Eq. (11.120) leads to the Ostrogradski instability with the Hamiltonian unbounded from below. This originates from the linear term $P_1Q_2 (= P_1\dot{q})$ in the Hamiltonian.

The term $\beta\dot{q}^2\ddot{q}$ in the Lagrangian (11.116) contributes to neither the background equation (11.117) nor the Hamiltonian (11.120). In fact, after integration by parts, we find that this is merely a boundary term irrelevant to the particle dynamics. Hence there are cases in which the Lagrangian containing derivatives higher than first order does not give rise to the propagation of extra degrees of freedom.

In the above discussion we focused on the time-dependent background, but in the four-dimensional spacetime physical quantities like a scalar field ϕ depend on the three-dimensional position $\mathbf{x}$ as well as time t . In the four-dimensional Minkowski spacetime, it may be possible to construct Lagrangians containing derivatives higher than first order, while the equations of motion are of second order. As we will discuss in Sec. 11.3.2, the Galileon corresponds to such a specific example.

11.3.2. Minkowski Galileons

The Galileon is a scalar field whose equation of motion respects the Galilean symmetry (11.102) in the Minkowski spacetime [50, 51]. By construction, the Galileon equation of motion is of second order, so there is no Ostrogradski instability. In the following, we review the construction of the Galileon Lagrangian in the four-dimensional Minkowski spacetime.

Let us consider the action $S = \int d^4x \mathcal{L}$ with the Lagrangian density

$$\mathcal{L} = \mathcal{A}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n} \partial_{\mu_1} \partial_{\nu_1} \phi \cdots \partial_{\mu_n} \partial_{\nu_n} \phi, \quad (11.121)$$

which contains the n products of second-order derivatives $\partial_{\mu_i} \partial_{\nu_i} \phi$. The tensor $\mathcal{A}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n}$ is totally anti-symmetric in its first n indices (associated with μ_i) and also separately in its last n indices (associated with ν_i). It also depends on ϕ and its first derivative $\partial_\mu \phi$ alone, i.e.,

$$\mathcal{A}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n} = \mathcal{A}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n}(\phi, \partial_\mu \phi). \quad (11.122)$$

The Minkowski Galileon corresponds to the choice [63]

$$\mathcal{A}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n} = \mathcal{B}_{(2n+2)}^{\mu_1 \cdots \mu_{n+1} \nu_1 \cdots \nu_{n+1}} \partial_{\mu_{n+1}} \phi \partial_{\nu_{n+1}} \phi, \quad (11.123)$$

where

$$\mathcal{B}_{(2m)}^{\mu_1 \cdots \mu_m \nu_1 \cdots \nu_m} \equiv \frac{1}{(4-m)!} \varepsilon^{\mu_1 \cdots \mu_m \lambda_1 \cdots \lambda_{4-m}} \varepsilon^{\nu_1 \cdots \nu_m \lambda_1 \cdots \lambda_{4-m}}. \quad (11.124)$$

The lower index $2m$ represents the number of contravariant components, and ε is the totally anti-symmetric Levi-Civita tensor defined by Eq. (9.42). In the Minkowski spacetime, the Levi-Civita tensor simply reduces to $\varepsilon_{\mu\nu\rho\sigma} = \bar{\varepsilon}_{\mu\nu\rho\sigma}$, so that $\varepsilon_{0123} = 1$, $\varepsilon_{1023} = -1$, and $\varepsilon^{0123} = -1$ etc. It is also convenient to notice the following relations

$$\begin{aligned} \varepsilon^{\mu\nu\rho\sigma} \varepsilon_{\mu\nu\rho\sigma} &= -4!, & \varepsilon^{\alpha\nu\rho\sigma} \varepsilon_{\mu\nu\rho\sigma} &= -3! \delta_\mu^\alpha, & \varepsilon^{\alpha\beta\rho\sigma} \varepsilon_{\mu\nu\rho\sigma} &= -(2!)^2 \delta_\mu^{[\alpha} \delta_\nu^{\beta]}, \\ \varepsilon^{\alpha\beta\gamma\sigma} \varepsilon_{\mu\nu\rho\sigma} &= -3! \delta_\mu^{[\alpha} \delta_\nu^\beta \delta_\rho^{\gamma]}, & \varepsilon^{\alpha\beta\gamma\delta} \varepsilon_{\mu\nu\rho\sigma} &= -4! \delta_\mu^{[\alpha} \delta_\nu^\beta \delta_\rho^\gamma \delta_\sigma^{\delta]}. \end{aligned} \quad (11.125)$$

The square bracket represents the anti-symmetric permutation of a n -rank tensor $C^{\mu_1 \cdots \mu_n}$, such that

$$C^{[\mu_1 \cdots \mu_n]} = \frac{1}{n!} \sum_{\text{permutation}} (-)^P C^{\mu_1 \cdots \mu_n}, \quad (11.126)$$

where $(-)^P = 1$ for an even permutation and $(-)^P = -1$ for an odd permutation. If $n = 3$, for example, $C^{[\mu_1 \mu_2 \mu_3]} = (C^{\mu_1 \mu_2 \mu_3} + C^{\mu_2 \mu_3 \mu_1} + C^{\mu_3 \mu_1 \mu_2} - C^{\mu_2 \mu_1 \mu_3} - C^{\mu_1 \mu_3 \mu_2} - C^{\mu_3 \mu_2 \mu_1})/3!$.

From Eqs. (11.121) and (11.123) the Galileon Lagrangian density is given by

$$\mathcal{L}_N^{\text{Ga}} = \mathcal{B}_{(2n+2)}^{\mu_1 \cdots \mu_{n+1} \nu_1 \cdots \nu_{n+1}} \partial_{\mu_{n+1}} \phi \partial_{\nu_{n+1}} \phi \partial_{\mu_1} \partial_{\nu_1} \phi \cdots \partial_{\mu_n} \partial_{\nu_n} \phi, \quad (11.127)$$

which contains the $N = n + 2$ products of field derivatives. In four spacetime dimensions, the number of indices in $\mathcal{B}$ is restricted to be $n + 1 \leq 4$, so there are only four Galileon Lagrangians ($n = 0, 1, 2, 3$). On using the relations (11.125), they are given, respectively, by

$$\begin{aligned} \mathcal{L}_2^{\text{Ga}} &= \mathcal{B}_{(2)}^{\mu_1 \nu_1} \partial_{\mu_1} \phi \partial_{\nu_1} \phi \\ &= -\partial_\mu \phi \partial^\mu \phi, \end{aligned} \quad (11.128)$$

$$\begin{aligned} \mathcal{L}_3^{\text{Ga}} &= \mathcal{B}_{(4)}^{\mu_1 \mu_2 \nu_1 \nu_2} \partial_{\mu_2} \phi \partial_{\nu_2} \phi \partial_{\mu_1} \partial_{\nu_1} \phi \\ &= -(\partial_\mu \phi \partial^\mu \phi) \square \phi + \partial^\mu \phi \partial^\nu \phi \partial_\mu \partial_\nu \phi, \end{aligned} \quad (11.129)$$

$$\begin{aligned} \mathcal{L}_4^{\text{Ga}} &= \mathcal{B}_{(6)}^{\mu_1 \mu_2 \mu_3 \nu_1 \nu_2 \nu_3} \partial_{\mu_3} \phi \partial_{\nu_3} \phi \partial_{\mu_1} \partial_{\nu_1} \phi \partial_{\mu_2} \partial_{\nu_2} \phi \\ &= -(\partial_\mu \phi \partial^\mu \phi) (\square \phi)^2 + 2(\partial_\mu \phi \partial_\nu \phi \partial^\mu \partial^\nu \phi) \square \phi \\ &\quad + (\partial_\lambda \phi \partial^\lambda \phi) (\partial_\mu \partial_\nu \phi \partial^\mu \partial^\nu \phi) - 2\partial_\mu \phi \partial^\rho \phi \partial^\nu \partial^\mu \phi \partial_\rho \partial_\nu \phi, \end{aligned} \quad (11.130)$$

$$\begin{aligned} \mathcal{L}_5^{\text{Ga}} &= \mathcal{B}_{(8)}^{\mu_1 \mu_2 \mu_3 \mu_4 \nu_1 \nu_2 \nu_3 \nu_4} \partial_{\mu_4} \phi \partial_{\nu_4} \phi \partial_{\mu_1} \partial_{\nu_1} \phi \partial_{\mu_2} \partial_{\nu_2} \phi \partial_{\mu_3} \partial_{\nu_3} \phi \\ &= -(\partial_\mu \phi \partial^\mu \phi) (\square \phi)^3 + 3(\partial_\mu \phi \partial_\nu \phi \partial^\mu \partial^\nu \phi) (\square \phi)^2 + 3(\partial_\mu \partial_\nu \phi \partial^\mu \partial^\nu \phi) (\partial_\lambda \phi \partial^\lambda \phi) \square \phi \\ &\quad - 6(\partial_\mu \phi \partial^\rho \phi \partial^\nu \partial^\mu \phi \partial_\rho \partial_\nu \phi) \square \phi - 2(\partial_\rho \phi \partial^\rho \phi) (\partial^\nu \partial_\mu \phi \partial^\rho \partial_\nu \phi \partial^\mu \partial_\rho \phi) \\ &\quad - 3(\partial_\mu \partial_\nu \phi \partial^\mu \partial^\nu \phi) (\partial_\lambda \phi \partial_\rho \phi \partial^\lambda \partial^\rho \phi) + 6\partial_\mu \phi \partial_\lambda \phi \partial^\nu \partial^\mu \phi \partial_\rho \partial_\nu \phi \partial^\lambda \partial^\rho \phi, \end{aligned} \quad (11.131)$$

where $\square \phi \equiv \partial_\lambda \partial^\lambda \phi$.

The equation of motion following from the Lagrangian density (11.121) is $\mathcal{E} = 0$, where

$$\mathcal{E} \equiv \frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\mu \phi)} \right) + \partial_\mu \partial_\nu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\mu \partial_\nu \phi)} \right). \quad (11.132)$$

The term $\partial_\mu \partial_\nu (\partial \mathcal{L} / \partial (\partial_\mu \partial_\nu \phi))$ generally gives rise to derivatives up to fourth order. On using the anti-symmetric property of the tensor $\mathcal{A}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n}$ and the fact that the partial derivatives commute on the Minkowski spacetime, most of the terms containing the two subscripts of μ_i or ν_i (such as $\mathcal{A}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n} \cdots \partial_\mu \partial_\nu \partial_{\mu_k} \partial_{\nu_k} \phi \cdots$ and $\mathcal{A}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n} \cdots \partial_\nu \partial_{\mu_l} \partial_{\nu_l} \phi \partial_\mu \partial_{\mu_k} \partial_{\nu_k} \phi \cdots$) vanish. There is a non-vanishing third-order derivative

$$\frac{\partial \mathcal{A}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n}}{\partial (\partial_\alpha \phi)} \partial_\mu \partial_\nu \partial_\alpha \phi \partial_{\mu_1} \partial_{\nu_1} \phi \cdots \partial_{\mu_k} \partial_{\nu_k} \phi \cdots, \quad (11.133)$$

which arises from the third term in Eq. (11.132). However, it exactly cancels with the third-order derivative arising from the term $-\partial_\mu (\partial \mathcal{L} / \partial (\partial_\mu \phi))$. Hence we are left with only the second-order derivative terms in Eq. (11.132). Thus, the Lagrangian

(11.121) expressed in terms of the totally anti-symmetric tensor allows one to construct second-order theories for the scalar field ϕ [63].

For concreteness, let us consider the Galileon Lagrangian density (11.127). From the above discussion the equation of motion for each $N = n + 2$ is $\mathcal{E}_N = 0$, where

$$\mathcal{E}_N = -\mathcal{B}_{(2n+2)}^{\mu_1 \cdots \mu_{n+1} \nu_1 \cdots \nu_{n+1}} \partial_{\mu_1} \partial_{\nu_1} \phi \partial_{\mu_2} \partial_{\nu_2} \phi \cdots \partial_{\mu_{n+1}} \partial_{\nu_{n+1}} \phi. \quad (11.134)$$

Obviously this equation is invariant under the Galilean shift (11.102). The explicit forms of $\mathcal{E}_N$ (with $N = 2, 3, 4, 5$) are given by

$$\mathcal{E}_2 = \square \phi, \quad (11.135)$$

$$\mathcal{E}_3 = (\square \phi)^2 - \partial^\mu \partial^\nu \phi \partial_\mu \partial_\nu \phi, \quad (11.136)$$

$$\mathcal{E}_4 = (\square \phi)^3 - 3(\partial_\mu \partial_\nu \phi)(\partial^\mu \partial^\nu \phi) \square \phi + 2\partial^\mu \partial_\nu \phi \partial^\nu \partial_\lambda \phi \partial^\lambda \partial_\mu \phi, \quad (11.137)$$

$$\begin{aligned} \mathcal{E}_5 = & (\square \phi)^4 - 6\partial^\mu \partial^\nu \phi \partial_\mu \partial_\nu \phi + 3(\partial^\mu \partial^\nu \phi \partial_\mu \partial_\nu \phi)^2 \\ & + 8(\partial_\nu \partial^\mu \phi \partial_\rho \partial^\nu \phi \partial_\mu \partial^\rho \phi) \square \phi - 6\partial_\nu \partial^\mu \phi \partial_\rho \partial^\nu \phi \partial_\sigma \partial^\rho \phi \partial_\mu \partial^\sigma \phi. \end{aligned} \quad (11.138)$$

The Galileon Lagrangian density contains the first and second derivatives of ϕ . There is another Galilean invariant Lagrangian density characterized by the linear scalar potential:

$$\mathcal{L}_1^{\text{Ga}} = \phi, \quad (11.139)$$

in which case we have

$$\mathcal{E}_1 = 1. \quad (11.140)$$

The Galileon Lagrangian higher than the quintic order $\mathcal{L}_5^{\text{Ga}}$ does not exist, reflecting the fact that the totally anti-symmetric tensor (11.124) runs out of indices for $m > 4$. Thus, the full action of the Minkowski Galileon is given by

$$S = \int d^4x \sum_{N=1}^5 c_N \mathcal{L}_N^{\text{Ga}}, \quad (11.141)$$

where c_N 's are arbitrary constants.

The cubic term $\mathcal{L}_3^{\text{Ga}}$ reduces to $-(3/2)(\partial_\mu \phi \partial^\mu \phi) \square \phi \propto (\partial_\mu \phi \partial^\mu \phi) \mathcal{E}_2$ after the integration by parts. The quartic term $\mathcal{L}_4^{\text{Ga}}$ is equivalent to $-2(\partial_\mu \phi \partial^\mu \phi)[(\square \phi)^2 - \partial^\mu \partial^\nu \phi \partial_\mu \partial_\nu \phi] \propto (\partial_\mu \phi \partial^\mu \phi) \mathcal{E}_3$. The similar properties also hold for $N = 2, 5$, so the Galileon Lagrangian densities can be expressed in the form

$$\tilde{\mathcal{L}}_N^{\text{Ga}} = -2X \mathcal{E}_{N-1} \quad (11.142)$$

$$= -2\mathcal{B}_{(2n)}^{\mu_1 \cdots \mu_n \nu_1 \cdots \nu_n} X \partial_{\mu_1} \partial_{\nu_1} \phi \cdots \partial_{\mu_n} \partial_{\nu_n} \phi, \quad (11.143)$$

where $N = 2, 3, 4, 5$, and

$$X \equiv -\frac{1}{2}\partial_\mu\phi\partial^\mu\phi. \quad (11.144)$$

The Galileon is one of the examples of second-order scalar-field theories. In Ref. [64] it was shown that most general scalar theories with field equations containing derivatives up to second order are given by the sum of the Lagrangian densities $f_N(\phi, X)\tilde{\mathcal{L}}_N^{\text{Ga}}$ with $N = 2, 3, 4, 5$, where $f_N(\phi, X)$ are arbitrary functions of ϕ and X . Defining the function $g_N(\phi, X) \equiv -2Xf_N(\phi, X)$, the action of most general scalar theories with second-order equations of motion can be expressed as

$$S = \int d^4x \sum_{N=2}^5 \mathcal{L}_N, \quad \mathcal{L}_N \equiv g_N(\phi, X)\mathcal{E}_{N-1}. \quad (11.145)$$

Each Lagrangian density is given by

$$\mathcal{L}_2 = g_2(\phi, X), \quad (11.146)$$

$$\mathcal{L}_3 = g_3(\phi, X)\square\phi, \quad (11.147)$$

$$\mathcal{L}_4 = g_4(\phi, X) [(\square\phi)^2 - \partial^\mu\partial^\nu\phi\partial_\mu\partial_\nu\phi], \quad (11.148)$$

$$\mathcal{L}_5 = g_5(\phi, X) [(\square\phi)^3 - 3(\partial_\mu\partial_\nu\phi)(\partial^\mu\partial^\nu\phi)\square\phi + 2\partial^\mu\partial_\nu\phi\partial^\nu\partial_\lambda\phi\partial^\lambda\partial_\mu\phi]. \quad (11.149)$$

Since $\mathcal{L}_2$ has the ϕ dependence, the linear potential (11.139) in $\mathcal{L}_1$ can be absorbed into the definition of $\mathcal{L}_2$. The Galileon corresponds to the constant functions f_N , so that $g_{2,3,4,5} \propto X$. If we extend the action (11.145) to that on the curved space-time by keeping the second-order property, this gives rise to non-minimal derivative couplings between the scalar field ϕ and the gravity sector [64]. Such second-order theories are known as Horndeski theories [65]. We will discuss the action of Horndeski theories in Sec. 12.1.

11.3.3. Covariant Galileons

We now extend the Minkowski Galileon to that in the curved spacetime. If we promote partial derivatives to covariant derivatives for the first three Galileon terms in Eqs. (11.139) and (11.142), it follows that

$$\mathcal{L}_1^{\text{Ga,co}} = \phi, \quad (11.150)$$

$$\mathcal{L}_2^{\text{Ga,co}} = \nabla_\mu\phi\nabla^\mu\phi, \quad (11.151)$$

$$\mathcal{L}_3^{\text{Ga,co}} = (\nabla_\mu\phi\nabla^\mu\phi)\square\phi, \quad (11.152)$$

where $\square\phi = \nabla_\lambda\nabla^\lambda\phi$. The equations of motion following from $\mathcal{L}_2^{\text{Ga,co}}$ and $\mathcal{L}_3^{\text{Ga,co}}$ do not generally respect the Galilean symmetry (11.102) on the curved background. For example, let us consider the Lagrangian density $\mathcal{L} = -\nabla_\mu\phi\nabla^\mu\phi/2 - M^3\phi$,

where M is a constant having a dimension of mass. In this case, the field equation of motion is

$$\nabla^\mu \nabla_\mu \phi - M^3 = 0. \quad (11.153)$$

Under the Galilean shift (11.102), the covariant derivative $\nabla^\mu b_\mu$ does not vanish due to the presence of a non-vanishing Christoffel symbol.

Even if the Galilean symmetry is broken for $\mathcal{L}_2^{\text{Ga,co}}$ and $\mathcal{L}_3^{\text{Ga,co}}$, the field equations of motion are still of second order. If the field equations of motion are of second order on general curved backgrounds and the Galilean symmetry is recovered in the limit of Minkowski spacetime, such a scalar field is called ‘‘covariant Galileon’’ [53].

Although the covariantizations up to the cubic-order Galileon Lagrangians do not generate derivatives higher than second order, this is not the case for the quartic and quintic Lagrangians. Let us consider the quartic-order action

$$\begin{aligned} \mathcal{S}_4^{\text{Ga}} = \int d^4x \sqrt{-g} [& -(\nabla_\mu \phi \nabla^\mu \phi)(\square\phi)^2 + 2(\nabla_\mu \phi \nabla_\nu \phi \nabla^\mu \nabla^\nu \phi) \square\phi \\ & + (\nabla_\lambda \phi \nabla^\lambda \phi)(\nabla_\mu \nabla_\nu \phi \nabla^\mu \nabla^\nu \phi) - 2\nabla_\mu \phi \nabla^\rho \phi \nabla^\nu \nabla^\mu \phi \nabla_\rho \nabla_\nu \phi], \end{aligned} \quad (11.154)$$

which was derived by promoting partial derivatives in Eq. (11.130) to covariant derivatives. Varying the action (11.154) with respect to ϕ , we obtain the equation of motion $\mathcal{E}_4^{\text{Ga}} = 0$, where¹

$$\begin{aligned} \mathcal{E}_4^{\text{Ga}} = & (\square\phi)^3 - 3(\nabla_\mu \nabla_\nu \phi)(\nabla^\mu \nabla^\nu \phi) \square\phi + 2\nabla^\mu \nabla_\nu \phi \nabla^\nu \nabla_\lambda \phi \nabla^\lambda \nabla_\mu \phi \\ & - \frac{5}{2}(\square\phi) \nabla^\mu \phi (\nabla^\nu \nabla_\nu \nabla_\mu \phi - \nabla_\mu \nabla^\nu \nabla_\nu \phi) \\ & - 3\nabla_\mu \phi \nabla^\nu \nabla^\mu \phi (\nabla_\nu \nabla^\lambda \nabla_\lambda \phi - \nabla^\lambda \nabla_\lambda \nabla_\nu \phi) \\ & - 2\nabla^\mu \phi \nabla^\lambda \nabla^\nu \phi (\nabla_\mu \nabla_\lambda \nabla_\nu \phi - \nabla_\lambda \nabla_\nu \nabla_\mu \phi) \\ & - \frac{1}{2}(\nabla_\mu \phi \nabla^\mu \phi) (\nabla^\lambda \nabla_\lambda \nabla^\nu \nabla_\nu \phi - \nabla^\lambda \nabla^\nu \nabla_\lambda \nabla_\nu \phi) \\ & - \frac{1}{2} \nabla^\mu \phi \nabla^\nu \phi (2\nabla^\lambda \nabla_\nu \nabla_\lambda \nabla_\mu \phi - \nabla^\lambda \nabla_\lambda \nabla_\nu \nabla_\mu \phi - \nabla_\nu \nabla_\mu \nabla^\lambda \nabla_\lambda \phi). \end{aligned} \quad (11.155)$$

The first three terms contain second-order derivatives, which correspond to the covariantizations of Eq. (11.137). The other terms in Eq. (11.155) contain either third-order or fourth-order derivatives. The terms higher than second order can be

¹The equation of motion can be derived by using the xTensor written in the Wolfram language. The reader can download the xTensor package from the webpage: <http://xact.es/download.html>.

expressed in terms of curvature quantities, so Eq. (11.155) reduces to

$$\begin{aligned}
\mathcal{E}_4^{\text{Ga}} = & (\Box\phi)^3 - 3(\nabla_\mu\nabla_\nu\phi)(\nabla^\mu\nabla^\nu\phi)\Box\phi + 2\nabla^\mu\nabla_\nu\phi\nabla^\nu\nabla_\lambda\phi\nabla^\lambda\nabla_\mu\phi \\
& + \frac{1}{4}(\nabla_\mu\phi\nabla^\mu\phi)\nabla_\nu\phi\nabla^\nu R - \frac{5}{2}(\Box\phi)\nabla_\mu\phi R^{\mu\nu}\nabla_\nu\phi \\
& + 2\nabla_\mu\phi\nabla^\nu\nabla^\mu\phi R_{\nu\lambda}\nabla^\lambda\phi - \frac{1}{2}\nabla_\mu\phi\nabla_\nu\phi\nabla_\lambda\phi\nabla^\lambda R^{\mu\nu} \\
& + \frac{1}{2}(\nabla_\mu\phi\nabla^\mu\phi)\nabla_\lambda\nabla_\nu\phi R^{\nu\lambda} + 2\nabla_\mu\phi\nabla_\nu\phi\nabla_\sigma\nabla_\rho\phi R^{\mu\rho\nu\sigma}. \quad (11.156)
\end{aligned}$$

In the Minkowski limit, this recovers the equation of motion (11.137). On curved backgrounds the terms after the second lines of Eq. (11.156) contain the derivatives of R and $R^{\mu\nu}$, so the equation of motion contains third-order derivatives of the metric. To eliminate such derivative terms, we consider a linear combination of non-minimal derivative couplings of the forms $\mathcal{L}_{4,1} = (\nabla_\lambda\phi\nabla^\lambda\phi)(\nabla_\mu\phi\nabla^\mu\phi)R$ and $\mathcal{L}_{4,2} = (\nabla_\lambda\phi\nabla^\lambda\phi)(\nabla_\mu\phi R^{\mu\nu}\nabla_\nu\phi)$. In fact, the Lagrangian density

$$\mathcal{L}_4^{\text{nd}} \equiv \frac{1}{2}\mathcal{L}_{4,1} - \mathcal{L}_{4,2} = -(\nabla_\lambda\phi\nabla^\lambda\phi)\nabla_\mu\phi\left(R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R\right)\nabla_\nu\phi \quad (11.157)$$

is a unique combination to get rid of all third-order derivatives in Eq. (11.156) [53]. The corresponding action is given by

$$S_4^{\text{nd}} = - \int d^4x \sqrt{-g} (\nabla_\lambda\phi\nabla^\lambda\phi)(\nabla_\mu\phi G^{\mu\nu}\nabla_\nu\phi). \quad (11.158)$$

The field equation derived by the variation of the action $S_4^{\text{Ga,co}} = S_4^{\text{Ga}} + S_4^{\text{nd}}$ with respect to ϕ reads $\mathcal{E}_4^{\text{Ga,co}} = 0$, where

$$\begin{aligned}
\mathcal{E}_4^{\text{Ga,co}} = & (\Box\phi)^3 - 3(\nabla_\mu\nabla_\nu\phi)(\nabla^\mu\nabla^\nu\phi)\Box\phi + 2\nabla^\mu\nabla_\nu\phi\nabla^\nu\nabla_\lambda\phi\nabla^\lambda\nabla_\mu\phi \\
& - \frac{1}{2}(\Box\phi)(\nabla_\mu\phi\nabla^\mu\phi)R - R\nabla_\mu\phi\nabla^\nu\nabla^\mu\phi\nabla_\nu\phi \\
& - 2(\Box\phi)(R^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi) + 4R_{\nu\lambda}\nabla_\mu\phi\nabla^\nu\nabla^\mu\phi\nabla^\lambda\phi \\
& + R^{\nu\lambda}(\nabla_\mu\phi\nabla^\mu\phi)\nabla_\lambda\nabla_\nu\phi + 2R^{\mu\rho\nu\sigma}\nabla_\mu\phi\nabla_\nu\phi\nabla_\sigma\nabla_\rho\phi, \quad (11.159)
\end{aligned}$$

which is of second order in both the derivatives of ϕ and $g_{\mu\nu}$. Existence of the first-order derivatives of ϕ breaks the Galilean symmetry, but in the Minkowski limit the equation of motion (11.159) is invariant under the Galilean shift (11.102). After integrations by parts, the quartic-order covariant Galileon Lagrangian $S_4^{\text{Ga,co}}$ can be expressed in the form $S_4^{\text{Ga,co}} = - \int d^4x \sqrt{-g} \mathcal{L}_4^{\text{Ga,co}}$, where

$$\mathcal{L}_4^{\text{Ga,co}} = (\nabla_\lambda\phi\nabla^\lambda\phi) \left[2(\Box\phi)^2 - 2\nabla_\mu\nabla_\nu\phi\nabla^\mu\nabla^\nu\phi - \frac{1}{2}(\nabla_\mu\phi\nabla^\mu\phi)R \right]. \quad (11.160)$$

As we will see in more general theories in Sec. 12.1, the variation of the action $S_4^{\text{Ga,co}}$ with respect to the metric $g_{\mu\nu}$ also gives rise to second-order gravitational

equations of motion in both the derivatives of ϕ and $g_{\mu\nu}$. Thus, adding the non-minimal derivative coupling (11.158) to the action (11.154) allows one to construct the covariant Galileon Lagrangian $\mathcal{L}_4^{\text{Ga,co}}$ whose equations of motion are of second order on general curved backgrounds.

Let us next consider the quintic-order Galileon action given by

$$S_5^{\text{Ga}} = \int d^4x \sqrt{-g} \mathcal{L}_5^{\text{Ga}}, \quad (11.161)$$

where $\mathcal{L}_5^{\text{Ga}}$ is the Lagrangian density derived by replacing partial derivatives in Eq. (11.131) with covariant derivatives. Varying this action with respect to ϕ , we find that the equation of motion does not contain the derivatives of ϕ higher than second order. However, third-order derivatives of $g_{\mu\nu}$ arise as first-order derivatives of curvature quantities. Such higher-order terms are given by the combination

$$\begin{aligned} & 3(\Box\phi)(\nabla_\mu\phi\nabla^\mu\phi)(\nabla_\nu\phi\nabla^\nu R) - 3(\nabla_\mu\phi\nabla_\nu\phi\nabla^\nu\nabla^\mu\phi)(\nabla_\lambda\phi\nabla^\lambda R) \\ & - 6(\Box\phi)(\nabla_\mu\phi\nabla_\nu\phi\nabla_\lambda\phi\nabla^\lambda R^{\mu\nu}) - 6(\nabla_\mu\phi\nabla^\mu\phi)(\nabla_\nu\phi\nabla_\lambda\nabla_\rho\phi\nabla^\nu R^{\rho\lambda}) \\ & + 12\nabla_\mu\phi\nabla_\nu\phi\nabla^\lambda\phi\nabla_\rho\nabla_\lambda\phi\nabla^\nu R^{\mu\rho} + 6\nabla_\mu\phi\nabla_\nu\phi\nabla_\rho\phi\nabla_\lambda\nabla_\sigma\phi\nabla^\rho R^{\mu\sigma\nu\lambda}. \end{aligned} \quad (11.162)$$

The unique combination of the additional action that gets rids of all these higher-order terms is given by [53]

$$\begin{aligned} S_5^{\text{nd}} = 3 \int d^4x \sqrt{-g} (\nabla_\lambda\phi\nabla^\lambda\phi) & \left[R^{\mu\rho\nu\sigma} \nabla_\mu\phi\nabla_\nu\phi\nabla_\sigma\nabla_\rho\phi - R^{\nu\rho}(\Box\phi)\nabla_\nu\phi\nabla_\rho\phi \right. \\ & \left. + 6R_{\rho\sigma}\nabla_\nu\phi\nabla^\sigma\phi\nabla^\rho\nabla^\nu\phi - \frac{5}{2}R\nabla_\nu\phi\nabla_\rho\phi\nabla^\rho\nabla^\nu\phi \right]. \end{aligned} \quad (11.163)$$

Varying the total action $S_5^{\text{Ga,co}} = S_5^{\text{Ga}} + S_5^{\text{nd}}$ with respect to $g_{\mu\nu}$, it follows that the gravitational equations are also of second order in the derivatives of $g_{\mu\nu}$ and ϕ . After integrations by parts, the total action can be expressed in the simple form $S_5^{\text{Ga,co}} = -(5/2) \int d^4x \sqrt{-g} \mathcal{L}_5^{\text{Ga,co}}$, where

$$\begin{aligned} \mathcal{L}_5^{\text{Ga,co}} = & (\nabla_\lambda\phi\nabla^\lambda\phi)[(\Box\phi)^3 - 3(\nabla_\mu\nabla_\nu\phi)(\nabla^\mu\nabla^\nu\phi)\Box\phi + 2\nabla^\mu\nabla_\nu\phi\nabla^\nu\nabla_\rho\phi\nabla^\rho\nabla_\mu\phi \\ & - 6G_{\nu\rho}\nabla_\mu\phi\nabla^\nu\nabla^\mu\phi\nabla^\rho\phi]. \end{aligned} \quad (11.164)$$

In the Minkowski limit, this reduces to the Lagrangian density $\tilde{\mathcal{L}}_5^{\text{Ga}}$ given by Eq. (11.142) with $N = 5$.

In summary, the full covariant Galileon action in the presence of the Einstein–Hilbert term and the matter fields Ψ_M yields

$$S^{\text{Ga,co}} = \int d^4x \sqrt{-g} \left[\frac{M_{\text{pl}}^2}{2} R + \frac{1}{2} \sum_{i=1}^5 c_i M^{3(2-i)} \mathcal{L}_i^{\text{Ga,co}} \right] + S_M(g_{\mu\nu}, \Psi_M), \quad (11.165)$$

where S_M is the matter action, c_i 's are dimensionless constants, M is a constant having a dimension of mass, and $\mathcal{L}_i^{\text{Ga,co}}$'s ($i = 1, 2, 3, 4, 5$) are the Lagrangian densities given by Eqs. (11.150)–(11.152), (11.160) and (11.164), respectively.

In Refs. [60, 66, 67], it was shown that covariant Galileons are not renormalizable to any loop order in perturbation theory, so that they can be treated classically. It is also possible to extend the above theory to more general cases like multi-Galileons [68] (which arise from co-dimension greater than one flat branes embedded in a flat background) and super-symmetric Galileons [69].

11.3.4. Galileon cosmology

We study the background cosmological dynamics for the covariant Galileon theory given by the action (11.165). In doing so, we consider the flat FLRW background described by the line element

$$ds^2 = -N^2(t) dt^2 + a^2(t) \delta_{ij} dx^i dx^j. \quad (11.166)$$

Varying the action (11.165) with respect to N and a respectively and setting $N = 1$ in the end, we obtain two independent gravitational equations of motion associated with the metrics g_{00} and g_{ii} . For the matter action S_M , we take into account a perfect fluid described by the k-essence scalar field χ as

$$S_M = \int d^4x \sqrt{-g} P(X), \quad X = -\frac{1}{2} g^{\mu\nu} \partial_\mu \chi \partial_\nu \chi. \quad (11.167)$$

Computing the action (11.165) for the time-dependent Galileon field $\phi(t)$, we obtain the action containing the time derivatives $\dot{N}, \ddot{a}, \ddot{\phi}$.² After integrating them by parts, the action reduces to

$$S^{\text{Ga,co}} = \int d^4x a^3 \left[-\frac{3M_{\text{pl}}^2 H^2}{N} + \frac{1}{2} N c_1 M^3 \phi - \frac{c_2 \dot{\phi}^2}{2N} + \frac{c_3 \dot{\phi}^3 H}{N^3 M^3} - \frac{9c_4 \dot{\phi}^4 H^2}{2N^5 M^6} + \frac{3c_5 \dot{\phi}^5 H^3}{N^7 M^9} + NP(X(N)) \right], \quad (11.168)$$

where $H = \dot{a}/a$, and P depends on N through $X = \dot{\chi}^2/(2N^2)$. The action (11.168) does not contain the time derivative of N , so the variation of Eq. (11.168) with respect to N gives rise to a constraint equation $\delta S^{\text{Ga,co}}/\delta N = 0$. This is generally

²The computation can be easily done with the Maple software.

called a Hamiltonian constraint, which corresponds to the (00) component of the gravitational equation. For the action (11.168) the Hamiltonian constraint, derived after setting $N = 1$, yields

$$3M_{\text{pl}}^2 H^2 = \rho_{\text{DE}} + \rho_M, \quad (11.169)$$

where

$$\rho_{\text{DE}} \equiv -\frac{c_1}{2}M^3\dot{\phi} - \frac{c_2}{2}\dot{\phi}^2 + \frac{3c_3}{M^3}H\dot{\phi}^3 - \frac{45c_4}{2M^6}H^2\dot{\phi}^4 + \frac{21c_5}{M^9}H^3\dot{\phi}^5, \quad (11.170)$$

and $\rho_M \equiv 2XP_{,X} - P$ is the matter density.

Variation of the action (11.168) with respect to a leads to

$$3M_{\text{pl}}^2 H^2 + 2M_{\text{pl}}^2 \dot{H} = -P_{\text{DE}} - P_M, \quad (11.171)$$

where

$$\begin{aligned} P_{\text{DE}} \equiv & \frac{c_1}{2}M^3\dot{\phi} - \frac{c_2}{2}\dot{\phi}^2 - \frac{c_3}{M^3}\dot{\phi}^2\ddot{\phi} + \frac{3c_4}{2M^6}\dot{\phi}^3[8H\ddot{\phi} + (3H^2 + 2\dot{H})\dot{\phi}] \\ & - \frac{3c_5}{M^9}H\dot{\phi}^4[5H\ddot{\phi} + 2(H^2 + \dot{H})\dot{\phi}], \end{aligned} \quad (11.172)$$

and $P_M = P$ is the matter pressure. For the matter fluid, we consider non-relativistic matter (energy density ρ_m , pressure $P_m = 0$) and radiation (energy density ρ_r , pressure $P_r = \rho_r/3$), such that

$$\rho_M = \rho_m + \rho_r, \quad P_M = \frac{1}{3}\rho_r. \quad (11.173)$$

Varying the action (11.168) with respect to ϕ , we obtain the field equation

$$\begin{aligned} & \left(c_2 - \frac{6c_3}{M^3}H\dot{\phi} + \frac{54c_4}{M^6}H^2\dot{\phi}^2 - \frac{60c_5}{M^9}H^3\dot{\phi}^3 \right) \ddot{\phi} - \left(\frac{3c_3}{M^3} - \frac{36c_4}{M^6}H\dot{\phi} + \frac{45c_5}{M^9}H^2\dot{\phi}^2 \right) \dot{H}\dot{\phi}^2 \\ & + \frac{1}{2}c_1M^3 + 3c_2H\dot{\phi} - \frac{9c_3}{M^3}H^2\dot{\phi}^2 + \frac{54c_4}{M^6}H^3\dot{\phi}^3 - \frac{45c_5}{M^9}H^4\dot{\phi}^4 = 0. \end{aligned} \quad (11.174)$$

The energy density ρ_{DE} and the pressure P_{DE} of the “dark” sector obey the continuity equation $\dot{\rho}_{\text{DE}} + 3H(\rho_{\text{DE}} + P_{\text{DE}}) = 0$. In fact, this is equivalent to the field equation (11.174), which also follows by combining Eq. (11.169) with Eq. (11.171). We define the dark energy equation of state w_{DE} and the effective equation of state w_{eff} , as $w_{\text{DE}} = P_{\text{DE}}/\rho_{\text{DE}}$ and $w_{\text{eff}} = -1 - 2\dot{H}/(3H^2)$, respectively.

Our interest is the case in which the late-time cosmic acceleration is realized by the field kinetic terms, so we set $c_1 = 0$ in the following discussion. From Eqs. (11.169) and (11.171), we observe that it is possible to realize de Sitter solutions ($H = H_{\text{dS}} = \text{constant}$) with $\dot{\phi} = \dot{\phi}_{\text{dS}} = \text{constant}$. We normalize the mass M to be $M^3 = M_{\text{pl}}H_{\text{dS}}^2$. For $H_{\text{dS}} \approx 10^{-60}M_{\text{pl}}$, the mass M is of the order of $M \approx 10^{-40}M_{\text{pl}}$.

On defining the dimensionless quantity $x_{\text{dS}} \equiv \dot{\phi}_{\text{dS}}/(H_{\text{dS}}M_{\text{pl}})$, Eqs. (11.169) and (11.171) lead to the following relations at the de Sitter solution:

$$c_2 x_{\text{dS}}^2 = 6 + 9\alpha - 12\beta, \quad (11.175)$$

$$c_3 x_{\text{dS}}^3 = 2 + 9\alpha - 9\beta, \quad (11.176)$$

where

$$\alpha \equiv c_4 x_{\text{dS}}^4, \quad \beta \equiv c_5 x_{\text{dS}}^5. \quad (11.177)$$

As we will see below, the coefficients of physical quantities and dynamical equations can be expressed in terms of α and β . The relations (11.175) and (11.176) are invariant under the rescalings $x_{\text{dS}} \rightarrow \gamma x_{\text{dS}}$ and $c_i \rightarrow c_i/\gamma^i$, where γ is a real constant. Then, the rescaled choices of c_N give the same physics.

To study the background cosmological dynamics, we introduce the following dimensionless variables [57, 58]:

$$r_1 \equiv \frac{\dot{\phi}_{\text{dS}} H_{\text{dS}}}{\dot{\phi} H}, \quad r_2 \equiv \frac{1}{r_1} \left(\frac{\dot{\phi}}{\dot{\phi}_{\text{dS}}} \right)^4, \quad (11.178)$$

which are both equivalent to 1 at the de Sitter solution. Defining the dark energy density parameter $\Omega_{\text{DE}} \equiv \rho_{\text{DE}}/(3M_{\text{pl}}^2 H^2)$, it follows that

$$\Omega_{\text{DE}} = -\frac{1}{2}(2 + 3\alpha - 4\beta)r_1^3 r_2 + (2 + 9\alpha - 9\beta)r_1^2 r_2 - \frac{15}{2}\alpha r_1 r_2 + 7\beta r_2. \quad (11.179)$$

Then, Eq. (11.169) can be written as $\Omega_{\text{DE}} + \Omega_m + \Omega_r = 1$, where $\Omega_m = \rho_m/(3M_{\text{pl}}^2 H^2)$ and $\Omega_r = \rho_r/(3M_{\text{pl}}^2 H^2)$.

The autonomous equations for the variables r_1 , r_2 , and Ω_r are given, respectively, by

$$\begin{aligned} r_1' &= \frac{1}{\Delta} (r_1 - 1) r_1 [r_1 (r_1(-3\alpha + 4\beta - 2) + 6\alpha - 5\beta) - 5\beta] \\ &\quad \times [2(\Omega_r + 9) + 3r_2(r_1^3(-3\alpha + 4\beta - 2) + 2r_1^2(9\alpha - 9\beta + 2) \\ &\quad - 15r_1\alpha + 14\beta)], \end{aligned} \quad (11.180)$$

$$\begin{aligned} r_2' &= -\frac{1}{\Delta} [r_2(6r_1^2(r_2(45\alpha^2 - 4(9\alpha + 2)\beta + 36\beta^2) - (\Omega_r - 7)(9\alpha - 9\beta + 2)) \\ &\quad - r_1^3(2(\Omega_r + 33)(3\alpha - 4\beta + 2) + 3r_2(15\alpha(9\alpha + 2) - 2(201\alpha + 89)\beta + 356\beta^2)) \\ &\quad - 3r_1\alpha(-28\Omega_r + 123r_2\beta + 36) + 10\beta(-11\Omega_r + 21r_2\beta - 3) \\ &\quad + 3r_1^4 r_2(9\alpha^2 - 30\alpha(4\beta + 1) + 2(2 - 9\beta)^2) + 3r_1^6 r_2(3\alpha - 4\beta + 2)^2 \\ &\quad + 3r_1^5 r_2(9\alpha - 9\beta + 2)(3\alpha - 4\beta + 2))], \end{aligned} \quad (11.181)$$

$$\Omega_r' = -\Omega_r \left(4 + \frac{2H'}{H} \right), \quad (11.182)$$

where a prime represents the derivative with respect to $\mathcal{N} = \ln a$, and

$$\begin{aligned} \Delta \equiv & 2r_1^4 r_2 [72\alpha^2 + 30\alpha(1 - 5\beta) + (2 - 9\beta)^2] + 4r_1^2 [9r_2(5\alpha^2 + 9\alpha\beta + (2 - 9\beta)\beta) \\ & + 2(9\alpha - 9\beta + 2)] + 4r_1^3 [-3r_2 (-2(15\alpha + 1)\beta + 3\alpha(9\alpha + 2) + 4\beta^2) \\ & - 3\alpha + 4\beta - 2] - 24r_1\alpha(16r_2\beta + 3) + 10\beta(21r_2\beta + 8). \end{aligned} \quad (11.183)$$

The Hubble parameter obeys the differential equation

$$\frac{H'}{H} = -\frac{5r_1'}{4r_1} - \frac{r_2'}{4r_2}. \quad (11.184)$$

The integrated solution to Eq. (11.182) can be written in the form $\Omega_r(\mathcal{N}) = \Omega_r^{(0)} e^{-4\mathcal{N}} H_0^2 / H^2(\mathcal{N})$, where $\Omega_r^{(0)}$ is today's value of Ω_r (i.e., at $\mathcal{N} = 0$).

11.3.4.1. Tracker solutions ($r_1 = 1$)

From Eq. (11.180), we find that there is a specific fixed point satisfying

$$r_1 = 1, \quad (11.185)$$

along which the field velocity grows as $\dot{\phi} \propto 1/H$ with the decrease of H . This corresponds to a tracker solution that attracts solutions with different initial conditions to a common trajectory [57, 58]. Along the tracker, the dark energy density parameter (11.179) is given by

$$\Omega_{\text{DE}} = r_2. \quad (11.186)$$

Substituting $r_1 = 1$ into Eqs. (11.181) and (11.182), respectively, we obtain

$$r_2' = \frac{2r_2(3 - 3r_2 + \Omega_r)}{1 + r_2}, \quad (11.187)$$

$$\Omega_r' = \frac{\Omega_r(\Omega_r - 1 - 7r_2)}{1 + r_2}, \quad (11.188)$$

which are independent of α and β . There exist the following three fixed points:

$$(A) \ (r_1, r_2, \Omega_r) = (1, 0, 1), \quad (11.189)$$

$$(B) \ (r_1, r_2, \Omega_r) = (1, 0, 0), \quad (11.190)$$

$$(C) \ (r_1, r_2, \Omega_r) = (1, 1, 0). \quad (11.191)$$

The points (A) and (B) can be realized during the radiation and matter eras, respectively (i.e., $\Omega_{\text{DE}} \ll 1$), whereas the point (C) corresponds to the de Sitter solution mentioned above.

The stabilities of the points (A), (B), (C) are known by considering linear perturbations δr_1 , δr_2 , and $\delta \Omega_r$ about them. Defining the vector $\delta \mathbf{r} = {}^t(\delta r_1, \delta r_2, \delta \Omega_r)$, the linear perturbation equations can be written in the form

$$\delta \mathbf{r}' = \mathcal{M} \delta \mathbf{r}, \quad (11.192)$$

where $\mathcal{M}$ is the 3×3 matrix. The perturbation δr_1 obeys the differential equation

$$\delta r_1' = -\frac{9 + \Omega_r + 3r_2}{2(1 + r_2)} \delta r_1, \quad (11.193)$$

which means that the tracker is stable along the r_1 direction in the regimes $0 \leq r_2 \leq 1$ and $\Omega_r \geq 0$. The eigenvalues of the matrix $\mathcal{M}$ for the points (A), (B), (C) are given, respectively, by

$$(A) \ (8, 1, -5), \quad (B) \ (6, -1, -9/2), \quad (C) \ (-3, -3, -4). \quad (11.194)$$

This shows that (A) and (B) are saddle, while (C) is stable. Hence the tracker evolves along the sequence of fixed points: (A) $\rightarrow$ (B) $\rightarrow$ (C).

Along the tracker, we have $\rho_{\text{DE}} = 3M^6/H^2$, $P_{\text{DE}} = -3M^6(2 + w_{\text{eff}})/H^2$, and

$$w_{\text{DE}} = -2 - w_{\text{eff}} = -\frac{\Omega_r + 6}{3(r_2 + 1)}, \quad w_{\text{eff}} = \frac{\Omega_r - 6r_2}{3(r_2 + 1)}. \quad (11.195)$$

During the cosmological sequence of radiation, matter, and de Sitter epochs, the dark energy equation of state and the effective equation of state evolve, respectively, as $w_{\text{DE}} = -7/3 \rightarrow -2 \rightarrow -1$ and $w_{\text{eff}} = 1/3 \rightarrow 0 \rightarrow -1$. In Fig. 11.3, we plot the evolution of w_{DE} for the tracker solution as a solid line. In the early cosmological epoch, w_{DE} is quite away from the cosmological constant value -1 .

One can derive analytical solutions to Ω_{DE} and Ω_r for the tracker. Since we have the relation $r_2'/r_2 = 8 + 2\Omega_r'/\Omega_r$ from Eqs. (11.187) and (11.188), it follows that

$$\Omega_{\text{DE}} = r_2 = c_1 a^8 \Omega_r^2, \quad (11.196)$$

where c_1 is an integration constant. Substituting this solution into Eq. (11.188) and integrating it with respect to $\mathcal{N}$, we obtain two branches of solutions. The cosmologically viable branch corresponds to

$$\Omega_r = \frac{c_2 a - 1 + \sqrt{1 - 2c_2 a + c_2^2 a^2 + 4c_1 a^8}}{2c_1 a^8}, \quad (11.197)$$

where c_2 is another integration constant. At early times ($a \ll 1$), we have $\Omega_r \simeq 1 + c_2 a$, so that $c_2 < 0$ for $\Omega_{\text{DE}} > 0$. The coefficients c_1 and c_2 are known by using

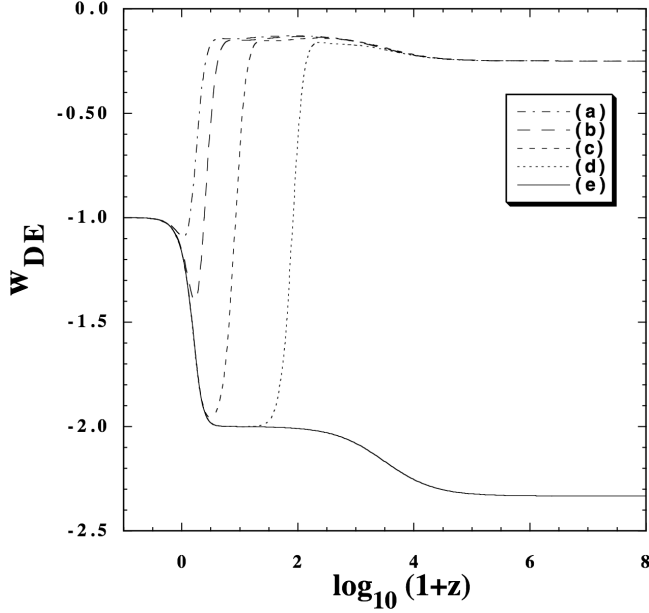


Fig. 11.3. Evolution of w_{DE} versus $z + 1 = 1/a$ for $\alpha = 0.3$ and $\beta = 0.14$ for the covariant Galileon model (11.165). We choose four different initial conditions: (a) $r_1 = 5.000 \times 10^{-11}$, $r_2 = 8.000 \times 10^{-12}$, and $\Omega_r = 0.999995$ at $z = 5.89 \times 10^8$, (b) $r_1 = 1.500 \times 10^{-10}$, $r_2 = 2.667 \times 10^{-12}$, and $\Omega_r = 0.999992$ at $z = 3.63 \times 10^8$, (c) $r_1 = 5.000 \times 10^{-9}$, $r_2 = 8.000 \times 10^{-14}$, and $\Omega_r = 0.99995$ at $z = 6.72 \times 10^7$, (d) $r_1 = 5.000 \times 10^{-6}$, $r_2 = 8.000 \times 10^{-17}$, and $\Omega_r = 0.9986$ at $z = 2.04 \times 10^6$. The thick line (e) corresponds to the tracker solution ($r_1 = 1$).

the density parameters of radiation and non-relativistic matter today ($a = 1$), as

$$c_1 = \frac{1 - \Omega_m^{(0)} - \Omega_r^{(0)}}{(\Omega_r^{(0)})^2}, \quad c_2 = -\frac{\Omega_m^{(0)}}{\Omega_r^{(0)}}. \quad (11.198)$$

Then, the density parameters Ω_{DE} , Ω_r , and $\Omega_m = 1 - \Omega_{\text{DE}} - \Omega_r$ as well as w_{DE} and w_{eff} are analytically known in terms of the function of a . Since the radiation density parameter has the dependence $\Omega_r \propto \rho_r/H^2 \propto 1/(a^4 H^2)$, we have that $H^2/H_0^2 = (\Omega_r^{(0)}/\Omega_r)(1/a^4)$. From Eq. (11.197), the Hubble parameter can be expressed in terms of the redshift $z = 1/a - 1$, as

$$\begin{aligned} \frac{H^2(z)}{H_0^2} &= \frac{1}{2}\Omega_m^{(0)}(1+z)^3 + \frac{1}{2}\Omega_r^{(0)}(1+z)^4 \\ &+ \sqrt{1 - \Omega_m^{(0)} - \Omega_r^{(0)} + \frac{(1+z)^6}{4} \left[\Omega_m^{(0)} + \Omega_r^{(0)}(1+z) \right]^2}. \end{aligned} \quad (11.199)$$

This analytic solution is useful to place observational constraints on the tracker. In Ref. [70], the authors confronted the covariant Galileon with the observational data of SN Ia, CMB shift parameters, and BAO. If the SN Ia data alone are used

in the likelihood analysis, the $\chi^2_{\text{SN Ia}}$ for the tracker is similar to that in the ΛCDM model. However, the combined data analysis of SN Ia+CMB+BAO shows that the difference of total χ^2 between the tracker and the ΛCDM model is $\delta\chi^2 \sim 22$ (which corresponds to 4.3σ). Hence the tracker is severely disfavored from the data relative to the ΛCDM model. The main reason for this incompatibility is attributed to the fact that the dark energy equation of state is away from -1 during the matter era ($w_{\text{DE}} = -2$).

11.3.4.2. Solutions before approaching the tracker ($r_1 \ll 1$)

Besides the tracker, there exists another solution before the system enters the tracking regime, i.e., $r_1 \ll 1$. Taking the limit $r_1 \rightarrow 0$ in Eq. (11.179), the dark energy density parameter is given by $\Omega_{\text{DE}} \simeq 7\beta r_2$. This is the regime in which the Lagrangian density $\mathcal{L}_5$ plays an important role for the cosmological dynamics. In the regime $r_1 \ll 1$, Eqs. (11.180) and (11.181) are approximately

$$r'_1 \simeq \frac{9 + \Omega_r + 21\beta r_2}{8 + 21\beta r_2} r_1, \quad r'_2 \simeq \frac{3 + 11\Omega_r - 21\beta r_2}{8 + 21\beta r_2} r_2. \quad (11.200)$$

Provided that $\Omega_{\text{DE}} \simeq 7\beta r_2 \ll 1$, these equations reduce, respectively, to $r'_1 \simeq (9 + \Omega_r)r_1/8$ and $r'_2 \simeq (3 + 11\Omega_r)r_2/8$. Hence the evolution of r_1 , r_2 , and $\dot{\phi}$ during the radiation and matter eras is given by

$$r_1 \propto a^{5/4}, \quad r_2 \propto a^{7/4}, \quad \dot{\phi} \propto t^{3/8}, \quad (\text{radiation era}), \quad (11.201)$$

$$r_1 \propto a^{9/8}, \quad r_2 \propto a^{3/8}, \quad \dot{\phi} \propto t^{1/4}, \quad (\text{matter era}). \quad (11.202)$$

The field velocity $\dot{\phi}$ grows more slowly compared to the tracker case (i.e., $\dot{\phi} \propto H^{-1} \propto t$). Since r_1 increases in time, the solutions eventually approach the tracker characterized by $r_1 = 1$.

In the regime $r_1 \ll 1$, the evolution of w_{DE} and w_{eff} is given, respectively, by

$$w_{\text{DE}} \simeq -\frac{1 + \Omega_r}{8 + 21\beta r_2}, \quad w_{\text{eff}} \simeq \frac{8\Omega_r - 21\beta r_2}{3(8 + 21\beta r_2)}. \quad (11.203)$$

As long as $\Omega_{\text{DE}} \ll 1$, we have that

$$w_{\text{DE}} \simeq -\frac{1}{4}, \quad w_{\text{eff}} \simeq \frac{1}{3}, \quad (\text{radiation era}), \quad (11.204)$$

$$w_{\text{DE}} \simeq -\frac{1}{8}, \quad w_{\text{eff}} \simeq 0, \quad (\text{matter era}). \quad (11.205)$$

This evolution of w_{DE} is quite different compared to that of the tracker solution.

In Fig. 11.3, we plot the evolution of w_{DE} for $\alpha = 0.3$ and $\beta = 0.14$ with several different initial conditions satisfying $r_1 \ll 1$. The dark energy equation of state starts to evolve from the value $w_{\text{DE}} \simeq -1/4$ in the radiation era. If the solutions do not yet reach the tracker at the end of the radiation era, w_{DE} approaches the value $-1/8$ during the matter dominance. Once the solutions reach the tracker

($r_1 = 1$), the evolution of w_{DE} is well described by Eq. (11.195). For smaller initial values of r_1 , the approach to the tracker occurs at later cosmological epochs.

In Ref. [70], the authors carried out the likelihood analysis for the initial conditions $r_1 \ll 1$ and showed that the solutions approaching the tracker at late times (such as the case (a) in Fig. 11.3) can be consistent with the combined data analysis of SN Ia, CMB, and BAO. In such cases, the total χ^2 has a similar value to that in the Λ CDM model. The early tracking (like the case (d) in Fig. 11.3) is disfavored from the data due to the large deviation of w_{DE} from -1 . Thus, the late-time tracking solution of covariant Galileons is allowed from the data at the expense of fine-tuned initial conditions.

We recall that the coefficients c_2 and c_3 are related to c_4 and c_5 as Eqs. (11.175) and (11.176) to realize de Sitter solutions. Without imposing these conditions among the coefficients, there exist other solutions relevant to the late-time cosmic acceleration. In such cases, as long as w_{DE} does not significantly deviate from -1 , the model can be also consistent with the observational data of SN Ia, CMB, and BAO [71].

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Chapter 12

Horndeski Theories and Cosmological Perturbations

In Sec. 11.3, we showed that the construction of second-order theories is important to avoid the Ostrogradski instability. The equations of motion of the Galileon field is of second order on the Minkowski background. If we simply replace partial derivatives of the Minkowski Galileon with covariant derivatives on the curved background, this gives rise to derivatives higher than second order. Adding gravitational counter terms to the action allows one to construct second-order theories in both the field and the metric. The similar prescription is also possible for a general single scalar field ϕ . Most general scalar–tensor theories with second-order equations of motion are known as Horndeski theories [1]. In this chapter, we will review Horndeski theories and its cosmological applications with the derivations of perturbation equations of motion as well as stability conditions. We will also apply our general results to place observational constraints on concrete modified gravity models of late-time cosmic acceleration from observations associated with the growth of inhomogeneities.

12.1. Horndeski theories

On the Minkowski background, most general second-order theories containing a single scalar field ϕ are given by the action (11.145). If we promote the Lagrangian densities (11.146)–(11.149) to those on the curved background by replacing partial derivatives with covariant derivatives, the quadratic and cubic Lagrangian densities $\mathcal{L}_2$ and $\mathcal{L}_3$ lead to second-order equations of motion in both ϕ and $g_{\mu\nu}$. However, this process gives rise to derivative terms higher than second order in the equations of motion arising from the quartic and quintic Lagrangian densities $\mathcal{L}_4$ and $\mathcal{L}_5$.

As in the case of covariant Galileons, it is possible to eliminate derivative terms higher than second order by adding non-minimal couplings to gravity. For the Lagrangian density $\mathcal{L}_4$, this amounts to adding the non-minimal coupling $G_4(\phi, X)R$

to Eq. (11.148) with the replacement $g_4(\phi, X) \rightarrow G_{4,X}(\phi, X) \equiv \partial G_4 / \partial X$ [2]. For $\mathcal{L}_5$, adding the gravitational coupling $G_5(\phi, X) G_{\mu\nu} \nabla^\mu \nabla^\nu \phi$ to Eq. (11.149) with the replacement $g_5(\phi, X) \rightarrow -G_{5,X}(\phi, X)/6$ leads to the second-order equations of motion in both ϕ and $g_{\mu\nu}$. In summary, the second-order generalization of the theories (11.145) to general curved backgrounds is given by the action

$$S^H = \int d^4x \sqrt{-g} \sum_{i=2}^5 \mathcal{L}_i, \quad (12.1)$$

where

$$\mathcal{L}_2 = G_2(\phi, X), \quad (12.2)$$

$$\mathcal{L}_3 = -G_3(\phi, X) \square \phi, \quad (12.3)$$

$$\mathcal{L}_4 = G_4(\phi, X) R + G_{4,X} [(\square \phi)^2 - (\nabla_\mu \nabla_\nu \phi) (\nabla^\mu \nabla^\nu \phi)], \quad (12.4)$$

$$\begin{aligned} \mathcal{L}_5 = G_5(\phi, X) G_{\mu\nu} (\nabla^\mu \nabla^\nu \phi) - \frac{1}{6} G_{5,X} [(\square \phi)^3 \\ - 3(\square \phi) (\nabla_\mu \nabla_\nu \phi) (\nabla^\mu \nabla^\nu \phi) + 2(\nabla^\mu \nabla_\nu \phi) (\nabla^\nu \nabla_\lambda \phi) (\nabla^\lambda \nabla_\mu \phi)], \end{aligned} \quad (12.5)$$

with

$$X \equiv -\frac{1}{2} g^{\mu\nu} \nabla_\mu \phi \nabla_\nu \phi, \quad \square \phi \equiv \nabla_\mu \nabla^\mu \phi. \quad (12.6)$$

Besides the single scalar field ϕ , there are two tensor polarizations arising from the gravity sector. The action (12.1) corresponds to most general scalar–tensor theories with second-order equations. This action was first derived by Horndeski in 1973 with a different form [1]. This pioneering work of Horndeski was not recognized much for a long time, but it was revived after 2011 as a result of the extension of covariant Galileons [2, 3]. The equivalence of the original Horndeski action to the action (12.1) was explicitly shown in Ref. [4].

The k-essence, which is inside the framework of GR, corresponds to $G_2 \neq 0$, $G_3 = 0$, $G_4 = M_{\text{pl}}^2/2$, $G_5 = 0$. The quintessence is a specific case of k-essence given by the function $G_2(\phi, X) = X - V(\phi)$. Horndeski theories (12.1) also cover a wide range of modified gravitational theories listed below.

(1) Brans–Dicke theory (including $f(R)$ gravity)

The Brans–Dicke theory [5] discussed in Sec. 11.2 is characterized by the functions

$$G_2 = \frac{M_{\text{pl}}^2 \omega_{\text{BD}} X}{\phi} - V(\phi), \quad G_3 = 0, \quad G_4 = \frac{M_{\text{pl}}^2}{2} \phi, \quad G_5 = 0, \quad (12.7)$$

where the field ϕ here is dimensionless. As we already showed in Sec. 11.2.1, the metric $f(R)$ gravity is a specific case of Brans–Dicke theory with the parameter $\omega_{\text{BD}} = 0$. The dilaton gravity [6], which is the low-energy effective string theory at tree level, corresponds to $\omega_{\text{BD}} = -1$.

(2) Non-minimally coupled theories

There are modified gravitational theories in which the scalar field ϕ has a non-minimal coupling with R in the form $-\xi\phi^2 R/2$ [7–11]. Such theories are given by the functions

$$G_2 = \omega(\phi)X - V(\phi), \quad G_3 = 0, \quad G_4 = \frac{M_{\text{pl}}^2}{2} - \frac{1}{2}\xi\phi^2, \quad G_5 = 0, \quad (12.8)$$

where $\omega(\phi)$ and $V(\phi)$ are functions of ϕ . Higgs inflation [12] corresponds to a canonical field ($\omega(\phi) = 1$) with the potential $V(\phi) = (\lambda/4)(\phi^2 - v^2)^2$.

(3) Covariant Galileons

The action (11.165) of covariant Galileons [13] corresponds to

$$\begin{aligned} G_2 &= \frac{1}{2}c_1 M^3 \phi - c_2 X, & G_3 &= \frac{c_3}{M^3} X, \\ G_4 &= \frac{M_{\text{pl}}^2}{2} - \frac{c_4}{M^6} X^2, & G_5 &= \frac{3c_5}{M^9} X^2. \end{aligned} \quad (12.9)$$

(4) Derivative couplings

There exists a theory of derivative couplings in which the field derivative $\nabla^\mu \phi$ is coupled to the Einstein tensor in the form $G_{\mu\nu} \nabla^\mu \phi \nabla^\nu \phi$ [14, 15]. After integration by parts, this coupling reduces to $-\phi G_{\mu\nu} (\nabla^\mu \nabla^\nu \phi)$. In the presence of the scalar potential $V(\phi)$ and the Einstein–Hilbert term $M_{\text{pl}}^2 R/2$, this theory corresponds to the choice

$$G_2 = X - V(\phi), \quad G_3 = 0, \quad G_4 = \frac{M_{\text{pl}}^2}{2}, \quad G_5 = c\phi, \quad (12.10)$$

where c is a constant.

(5) Gauss–Bonnet couplings

The Gauss–Bonnet term is defined by [16]

$$R_{\text{GB}}^2 \equiv R^2 - 4R_{\mu\nu}R^{\mu\nu} + R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma}. \quad (12.11)$$

In four-dimensional spacetime it reduces to a topological surface term, so it does not contribute to the equations of motion. If the scalar field ϕ is coupled to the Gauss–Bonnet term in the form $-\xi(\phi)R_{\text{GB}}^2$, where $\xi(\phi)$ is an arbitrary function of ϕ , this gives rise to a non-vanishing contribution to the equation of motion. This Gauss–Bonnet coupling $-\xi(\phi)R_{\text{GB}}^2$ can be accommodated by the choice [4]:

$$\begin{aligned} G_2 &= 8\xi^{(4)}(\phi)X^2(3 - \ln X), & G_3 &= 4\xi^{(3)}(\phi)X(7 - 3\ln X), \\ G_4 &= 4\xi^{(2)}(\phi)X(2 - \ln X), & G_5 &= -4\xi^{(1)}(\phi)\ln X, \end{aligned} \quad (12.12)$$

where $\xi^{(n)}(\phi) \equiv \partial^n \xi(\phi) / \partial \phi^n$.

The scalar field ϕ can be responsible for the cosmic acceleration depending on the functional forms of $G_{2,3,4,5}$. Since our interest is the application to dark energy,

we take into account matter fields Ψ_m (dark matter, baryons, radiation,...) to the Horndeski action (12.1). Namely, we focus on the theories given by the action

$$S = S^H + \int d^4x L_m(g_{\mu\nu}, \Psi_m), \quad (12.13)$$

where L_m is the matter Lagrangian. We assume that the matter sector does not have a direct coupling to ϕ , so that the matter energy-momentum tensor $T_{\mu\nu} = -(2/\sqrt{-g})\delta L_m/\delta g^{\mu\nu}$ obeys the continuity equation

$$\nabla^\mu T_{\mu\nu} = 0. \quad (12.14)$$

Varying the action (12.13) with respect to $g^{\mu\nu}$, it follows that [4]

$$\delta S_g = \int d^4x \sqrt{-g} \left(\sum_{i=2}^5 \mathcal{G}_{\mu\nu}^{(i)} - \frac{T_{\mu\nu}}{2} \right) \delta g^{\mu\nu}, \quad (12.15)$$

where the contributions $\mathcal{G}_{\mu\nu}^{(2)}, \mathcal{G}_{\mu\nu}^{(3)}, \mathcal{G}_{\mu\nu}^{(4)}, \mathcal{G}_{\mu\nu}^{(5)}$ come from the Lagrangian densities $\mathcal{L}_2, \mathcal{L}_3, \mathcal{L}_4, \mathcal{L}_5$, respectively. The explicit forms of these contributions are presented in Appendix A. The resulting gravitational equations of motion read

$$\sum_{i=2}^5 \mathcal{G}_{\mu\nu}^{(i)} = \frac{T_{\mu\nu}}{2}. \quad (12.16)$$

Variation of the action (12.13) with respect to ϕ leads to

$$\delta S_\phi = \int d^4x \sqrt{-g} \sum_{i=2}^5 \left(P_\phi^{(i)} - \nabla^\mu J_\mu^{(i)} \right) \delta \phi, \quad (12.17)$$

where the explicit forms of $P_\phi^{(i)}$ and $J_\mu^{(i)}$ are given in Appendix A. Then, the field equation of motion yields

$$\sum_{i=2}^5 \left(P_\phi^{(i)} - \nabla^\mu J_\mu^{(i)} \right) = 0. \quad (12.18)$$

The solutions to $g_{\mu\nu}$ and ϕ are known by solving Eqs. (12.16) and (12.18) for a given background.

12.2. Scalar cosmological perturbations in Horndeski theories

In Horndeski theories given by the action (12.1), we will derive linear perturbation equations of motion on the flat FLRW background in the presence of a matter perfect fluid. We assume that the perfect fluid is minimally coupled to gravity.

The background equations of motion can be derived by computing the quantities $\mathcal{G}_{\mu\nu}^{(i)}, P_\phi^{(i)}, J_\mu^{(i)}$ given in Appendix A for the line element $ds^2 = -dt^2 + a^2(t)\delta_{ij}dx^i dx^j$ and by substituting them into Eqs. (12.16) and (12.18). Alternatively, as we showed in Sec. 11.3.4 for covariant Galileons, we can compute the action (12.13) for the

metric (11.166) with the lapse function N and the scale factor a . Taking the latter procedure and varying the action with respect to N and a , the resulting gravitational equations of motion, derived after setting $N = 1$, are given, respectively, by

$$\begin{aligned}\mathcal{E} \equiv & 2XG_{2,X} - G_2 + 6X\dot{\phi}HG_{3,X} - 2XG_{3,\phi} \\ & - 6H^2G_4 + 24H^2X(G_{4,X} + XG_{4,XX}) - 12HX\dot{\phi}G_{4,\phi X} - 6H\dot{\phi}G_{4,\phi} \\ & + 2H^3X\dot{\phi}(5G_{5,X} + 2XG_{5,XX}) - 6H^2X(3G_{5,\phi} + 2XG_{5,\phi X}) = -\rho,\end{aligned}\quad (12.19)$$

$$\begin{aligned}\mathcal{P} \equiv & G_2 - 2X\left(G_{3,\phi} + \ddot{\phi}G_{3,X}\right) \\ & + 2\left(3H^2 + 2\dot{H}\right)G_4 - 4HG_{4,X}\left(\dot{X} + 3HX\right) - 8X\left(\dot{H}G_{4,X} + H\dot{X}G_{4,XX}\right) \\ & + 2\left(\ddot{\phi} + 2H\dot{\phi}\right)G_{4,\phi} + 4XG_{4,\phi\phi} + 4X\left(\ddot{\phi} - 2H\dot{\phi}\right)G_{4,\phi X} \\ & - 2X\left(2H^3\dot{\phi} + 2H\dot{H}\dot{\phi} + 3H^2\ddot{\phi}\right)G_{5,X} - 4H^2X^2\ddot{\phi}G_{5,XX} + 4HX\dot{\phi}G_{5,\phi\phi} \\ & + 2\left[2\left(\dot{H}X + H\dot{X}\right) + 3H^2X\right]G_{5,\phi} + 4HX\left(\dot{X} - HX\right)G_{5,\phi X} = -P,\end{aligned}\quad (12.20)$$

where ρ and P are the energy density and the pressure of the perfect fluid, respectively, satisfying the continuity equation

$$\dot{\rho} + 3H(\rho + P) = 0. \quad (12.21)$$

The field kinetic energy is equivalent to $X = \dot{\phi}^2/2$.

Variation of the action (12.13) with respect to ϕ gives

$$\frac{1}{a^3} \frac{d}{dt} (a^3 J_\phi) = P_\phi, \quad (12.22)$$

where

$$\begin{aligned}J_\phi \equiv & \dot{\phi}G_{2,X} + 6HXG_{3,X} - 2\dot{\phi}G_{3,\phi} + 6H^2\dot{\phi}(G_{4,X} + 2XG_{4,XX}) - 12HXG_{4,\phi X} \\ & + 2H^3X(3G_{5,X} + 2XG_{5,XX}) - 6H^2\dot{\phi}(G_{5,\phi} + XG_{5,\phi X}),\end{aligned}\quad (12.23)$$

$$\begin{aligned}P_\phi \equiv & G_{2,\phi} - 2X\left(G_{3,\phi\phi} + \ddot{\phi}G_{3,\phi X}\right) + 6\left(2H^2 + \dot{H}\right)G_{4,\phi} + 6H\left(\dot{X} + 2HX\right)G_{4,\phi X} \\ & - 6H^2XG_{5,\phi\phi} + 2H^3X\dot{\phi}G_{5,\phi X}.\end{aligned}\quad (12.24)$$

Among the four Eqs. (12.19)–(12.22), three of them are independent. In fact, it is possible to derive Eq. (12.22) by using other three equations of motion.

For the derivation of scalar perturbation equations of motion, we consider the perturbed line element on top of the FLRW background:

$$ds^2 = -(1 + 2\Psi)dt^2 + 2\chi_{|i}dtdx^i + a^2(t)(1 + 2\Phi)\delta_{ij}dx^i dx^j, \quad (12.25)$$

where Ψ , Φ , and χ are scalar metric perturbations. We have chosen the gauge in which the contribution of the form $E_{|ij}dx^i dx^j$ appearing in Eq. (6.13) vanishes. This fixes the spatial scalar part ξ of the gauge-transformation vector ξ^μ . The temporal part ξ^0 of the vector ξ^μ can be fixed by choosing another gauge condition, say,

$\chi = 0$ (Newtonian gauge). To derive the perturbation equations of motion valid for general gauges, it is convenient to keep the metric in the form (12.25) without fixing χ to be 0.

We decompose the scalar field ϕ into the background part $^{(b)}\phi(t)$ and the perturbed part $\delta\phi(t, \mathbf{x})$ as

$$\phi(t, \mathbf{x}) = ^{(b)}\phi(t) + \delta\phi(t, \mathbf{x}), \quad (12.26)$$

where we will omit the index “(b)” in the following. We also consider the density perturbation $\delta\rho(t, \mathbf{x})$ and the momentum perturbation $\delta q(t, \mathbf{x})$ of the perfect fluid. We introduce the density contrast δ and the velocity potential $\mathcal{V}$ as

$$\delta \equiv \frac{\delta\rho}{\rho}, \quad \mathcal{V} \equiv -\frac{\delta q}{\rho + P}. \quad (12.27)$$

The definition of $\mathcal{V}$ matches with that defined in Sec. 6.9, which is related to the velocity potential v introduced in Sec. 6.3 as $\mathcal{V} = -a(v + B)$ [see Eq. (6.214)]. The gauge-invariant matter perturbation is given by $\delta\rho_m \equiv \delta\rho - 3H\delta q = \delta\rho + 3H(\rho + P)\mathcal{V}$, so the gauge-invariant matter density contrast reads

$$\delta_m \equiv \frac{\delta\rho_m}{\rho} = \delta + 3H(1 + w)\mathcal{V}, \quad (12.28)$$

where $w \equiv P/\rho$.

We are interested in the cosmology where the field ϕ is responsible for the late-time acceleration, so we focus on the case of non-relativistic matter satisfying $w = 0$ and $\delta P = 0$. In other words, we focus on the cosmological evolution after the onset of the matter-dominated epoch. Since the perfect fluid is assumed to be minimally coupled to gravity, the perturbations δ and $\mathcal{V}$ obey the same equations of motion as those in GR. In Sec. 6.9, we already derived them by varying the Schutz–Sorkin action (6.203). Setting both P and c_M^2 to 0 in Eqs. (6.227) and (6.228), the matter perturbations in Fourier space obey

$$\dot{\delta} + 3\dot{\Phi} + \frac{k^2}{a^2}(\mathcal{V} + \chi) = 0, \quad (12.29)$$

$$\dot{\mathcal{V}} - \Psi = 0, \quad (12.30)$$

where k is a comoving wave number. Taking the time derivative of Eq. (12.29) and using Eq. (12.30), the gauge-invariant density contrast δ_m satisfies

$$\ddot{\delta}_m + 2H\dot{\delta}_m + \frac{k^2}{a^2}(\Psi + \dot{\chi}) = 3\left(\ddot{I} + 2H\dot{I}\right), \quad (12.31)$$

where $I \equiv H\mathcal{V} - \Phi$.

In order to study the perturbation equations of the gravity sector, it is convenient to introduce the following quantities:

$$w_1 \equiv 2(G_4 - 2XG_{4,X}) - 2X(G_{5,X}\dot{\phi}H - G_{5,\phi}), \quad (12.32)$$

$$w_2 \equiv -2G_{3,X}X\dot{\phi} + 4G_4H - 16X^2G_{4,XX}H + 4(\dot{\phi}G_{4,\phi X} - 4HG_{4,X})X + 2G_{4,\phi}\dot{\phi} \\ + 8X^2HG_{5,\phi X} + 2HX(6G_{5,\phi} - 5G_{5,X}\dot{\phi}H) - 4G_{5,XX}\dot{\phi}X^2H^2, \quad (12.33)$$

$$w_3 \equiv 3X(G_{2,X} + 2XG_{2,XX}) + 6X(3X\dot{\phi}HG_{3,XX} - G_{3,\phi X}X - G_{3,\phi} + 6H\dot{\phi}G_{3,X}) \\ + 18H(4HX^3G_{4,XXX} - HG_4 - 5X\dot{\phi}G_{4,\phi X} - G_{4,\phi}\dot{\phi} + 7HG_{4,X}X \\ + 16HX^2G_{4,XX} - 2X^2\dot{\phi}G_{4,\phi XX}) + 6H^2X(2H\dot{\phi}G_{5,XXX}X^2 - 6X^2G_{5,\phi XX} \\ + 13XH\dot{\phi}G_{5,XX} - 27G_{5,\phi X}X + 15H\dot{\phi}G_{5,X} - 18G_{5,\phi}), \quad (12.34)$$

$$w_4 \equiv 2G_4 - 2XG_{5,\phi} - 2XG_{5,X}\ddot{\phi}. \quad (12.35)$$

As we will see in Sec. 12.3, the quantities w_1 and w_4 are related to no-ghost and stability conditions of tensor perturbations. To discuss no-ghost and stability conditions of scalar perturbations, we also need to introduce the quantities w_2 and w_3 in addition to w_1 and w_4 .¹

Perturbing the gravitational equations (12.16) and the scalar-field equation (12.18) at linear order in perturbations, we can derive the gravitational equations of motion for Ψ, Φ, χ and the equation for the field perturbation $\delta\phi$. Alternatively, we expand the action (12.13) up to second order in scalar perturbations and vary the second-order action with respect to $\Psi, \Phi, \chi, \delta\phi$. In Sec. 12.3, we will address this issue with the Schutz–Sorkin matter action. In Fourier space, the linear perturbation equations are given, respectively, by [19]

$$E_\Psi \equiv A_1\dot{\Phi} + A_2\dot{\delta\phi} - \rho\dot{\mathcal{V}} + A_3\frac{k^2}{a^2}\Phi + A_4\Psi + A_5\frac{k^2}{a^2}\chi \\ + \left(A_6\frac{k^2}{a^2} - \mu\right)\delta\phi - \rho\delta = 0, \quad (12.36)$$

$$E_\Phi \equiv B_1\ddot{\Phi} + B_2\ddot{\delta\phi} + B_3\dot{\Phi} + B_4\dot{\delta\phi} + B_5\dot{\Psi} + B_6\frac{k^2}{a^2}\Phi + \left(B_7\frac{k^2}{a^2} + 3\nu\right)\delta\phi \\ + \left(B_8\frac{k^2}{a^2} + B_9\right)\Psi + B_{10}\frac{k^2}{a^2}\dot{\chi} + B_{11}\frac{k^2}{a^2}\chi + 3\rho\dot{\mathcal{V}} = 0, \quad (12.37)$$

$$E_\chi \equiv C_1\dot{\Phi} + C_2\dot{\delta\phi} + C_3\Psi + C_4\delta\phi + \rho\mathcal{V} = 0, \quad (12.38)$$

$$E_{\delta\phi} \equiv D_1\ddot{\Phi} + D_2\ddot{\delta\phi} + D_3\dot{\Phi} + D_4\dot{\delta\phi} + D_5\dot{\Psi} + D_6\frac{k^2}{a^2}\dot{\chi} + \left(D_7\frac{k^2}{a^2} + D_8\right)\Phi \\ + \left(D_9\frac{k^2}{a^2} - M_\phi^2\right)\delta\phi + \left(D_{10}\frac{k^2}{a^2} + D_{11}\right)\Psi + D_{12}\frac{k^2}{a^2}\chi = 0, \quad (12.39)$$

¹Compared to the notations used in Ref. [19], there are the correspondences: $w_1 = \mathcal{G}_T$, $w_2 = 2\Theta$, $w_3 = 3\Sigma$, and $w_4 = \mathcal{F}_T$.

where

$$\begin{aligned}
A_1 &= 3w_2, & A_2 &= -\frac{1}{3\dot{\phi}}(9Hw_2 + 2w_3), & A_3 &= 2w_1, & A_4 &= \frac{2}{3}w_3 + \rho, \\
A_5 &= w_2, & A_6 &= \frac{1}{\dot{\phi}}(w_2 - 2Hw_1), \\
B_1 &= 6w_1, & B_2 &= \frac{3}{\dot{\phi}}(w_2 - 2Hw_1), & B_3 &= 6(\dot{w}_1 + 3Hw_1), \\
B_4 &= \frac{3}{\dot{\phi}^2} \left[(4H\ddot{\phi} - 4\dot{H}\dot{\phi} - 6H^2\dot{\phi})w_1 - 2H\dot{\phi}\dot{w}_1 - (2\ddot{\phi} - 3H\dot{\phi})w_2 + \dot{\phi}\dot{w}_2 - \rho\dot{\phi} \right], \\
B_5 &= -3w_2, & B_6 &= 2w_4, & B_7 &= \frac{2}{\dot{\phi}}[\dot{w}_1 + H(w_1 - w_4)], & B_8 &= 2w_1, \\
B_9 &= -3(\dot{w}_2 + 3Hw_2), & B_{10} &= 2w_1, & B_{11} &= 2(\dot{w}_1 + Hw_1), \\
C_1 &= 2w_1, & C_2 &= \frac{1}{\dot{\phi}}(w_2 - 2Hw_1), & C_3 &= -w_2, \\
C_4 &= \frac{1}{\dot{\phi}^2} \left[2(H\ddot{\phi} - \dot{H}\dot{\phi})w_1 - \ddot{\phi}w_2 - \rho\dot{\phi} \right], \\
D_1 &= \frac{3}{\dot{\phi}}(w_2 - 2Hw_1), & D_2 &= \frac{2}{3\dot{\phi}^2}(9H^2w_1 - 9Hw_2 - w_3), \\
D_3 &= -\frac{3}{\dot{\phi}}[2H(\dot{w}_1 + 3Hw_1) - \dot{w}_2 - 3Hw_2 - \rho], \\
D_4 &= \frac{2}{\dot{\phi}^3} [3H\{(3H^2 + 2\dot{H})\dot{\phi} - 2H\ddot{\phi}\}w_1 + 3H^2\dot{\phi}\dot{w}_1 + 3\{2H\ddot{\phi} - (3H^2 + \dot{H})\dot{\phi}\}w_2 \\
&\quad - 3H\dot{\phi}\dot{w}_2 + \frac{1}{3}(2\ddot{\phi} - 3H\dot{\phi})w_3 - \frac{1}{3}\dot{\phi}\dot{w}_3], \\
D_5 &= \frac{1}{3\dot{\phi}}(9Hw_2 + 2w_3), & D_6 &= \frac{1}{\dot{\phi}}(w_2 - 2Hw_1), \\
D_7 &= \frac{2}{\dot{\phi}}[\dot{w}_1 + H(w_1 - w_4)], \\
D_8 &= \frac{3}{\dot{\phi}^2} \left[3(\dot{H}\dot{\phi} - H\ddot{\phi})w_2 - \frac{2}{3}\ddot{\phi}w_3 + 3H\rho\dot{\phi} - \mu\dot{\phi}^2 \right], \\
D_9 &= \frac{1}{\dot{\phi}^2} [2H^2w_4 - 4H(\dot{w}_1 + Hw_1) + \dot{w}_2 + Hw_2 + \rho], & D_{10} &= \frac{1}{\dot{\phi}}(w_2 - 2Hw_1), \\
D_{11} &= \frac{1}{\dot{\phi}^2} \left[3\{(3H^2 + \dot{H})\dot{\phi} - H\ddot{\phi}\}w_2 + 3H\dot{\phi}\dot{w}_2 + \frac{2}{3}(3H\dot{\phi} - \ddot{\phi})w_3 + \frac{2}{3}\dot{\phi}\dot{w}_3 - \mu\dot{\phi}^2 \right], \\
D_{12} &= -\frac{1}{\dot{\phi}} [2H(\dot{w}_1 + Hw_1) - \dot{w}_2 - Hw_2 - \rho], \tag{12.40}
\end{aligned}$$

and

$$\mu = \mathcal{E}_{,\phi}, \quad \nu = \mathcal{P}_{,\phi}, \quad M_\phi^2 = \frac{1}{\phi} [\dot{\mu} + 3H(\mu + \nu)]. \quad (12.41)$$

The quantities $\mathcal{E}$ and $\mathcal{P}$ are given, respectively, by Eqs. (12.19) and (12.20). In Appendix B, we present the explicit form of the term M_ϕ^2 , which contains the contribution $-G_{2,\phi\phi}$. For a canonical scalar field with the Lagrangian density $G_2 = X - V(\phi)$, this corresponds to the field mass squared $V_{,\phi\phi}$. For viable dark energy models in the framework of $f(R)$ gravity and Brans–Dicke theory, the term $V_{,\phi\phi}$ is the dominant contribution to M_ϕ^2 in the early cosmological epoch.

It is also convenient to notice the following relation

$$\frac{k^2}{a^2} E_\gamma \equiv 3 \left(\dot{E}_\chi + 3H E_\chi \right) - E_\Phi = 0, \quad (12.42)$$

where

$$E_\gamma \equiv B_6 \Phi + B_7 \delta\phi + B_8 \Psi + B_{10} \dot{\chi} + B_{11} \chi = 0. \quad (12.43)$$

This corresponds to the traceless part of the gravitational equations.

In the following, we choose the Newtonian gauge

$$\chi = 0. \quad (12.44)$$

Then, Eq. (12.43) becomes

$$B_6 \Phi + B_7 \delta\phi + B_8 \Psi = 0. \quad (12.45)$$

Since we are interested in the evolution of perturbations related to the observations of large-scale structures and weak lensing, we consider the modes deep inside the Hubble radius ($k^2/a^2 \gg H^2$). In this case, the terms containing k^2/a^2 give the dominant contribution to perturbation equations of motion. Strictly speaking this corresponds to the approximation $c_s^2 k^2/a^2 \gg H^2$, where c_s is the scalar sound speed which will be explicitly derived in Sec. 12.3. Moreover, we employ the quasi-static approximation under which the time-derivative terms such as those containing $\dot{\Phi}$, $\delta\dot{\phi}$, $\dot{\Psi}$ are neglected relative to the k^2 -dependent terms like $(k^2/a^2)\Phi$ [17–19]. This amounts to neglecting the oscillating mode of $\delta\phi$ relative to that of the matter-induced mode. We also keep the contribution of the term M_ϕ^2 , as it can be large in the early cosmological epoch in some of modified gravity models like $f(R)$ gravity [20–22] and Brans–Dicke theories [23].

Under this approximation scheme, Eqs. (12.36) and (12.39) reduce, respectively, to

$$B_8 \frac{k^2}{a^2} \Phi + A_6 \frac{k^2}{a^2} \delta\phi - \rho\delta \simeq 0, \quad (12.46)$$

$$B_7 \frac{k^2}{a^2} \Phi + \left(D_9 \frac{k^2}{a^2} - M_\phi^2 \right) \delta\phi + A_6 \frac{k^2}{a^2} \Psi \simeq 0, \quad (12.47)$$

where we used the properties $A_3 = B_8$, $D_7 = B_7$, and $D_{10} = A_6$. We can solve Eqs. (12.45)–(12.47) for $\delta\phi$, Ψ , Φ . Then, the field perturbation $\delta\phi$ yields

$$\delta\phi \simeq \frac{A_6 B_6 - B_7 B_8}{(A_6^2 B_6 + B_8^2 D_9 - 2A_6 B_7 B_8)(k/a)^2 - B_8^2 M_\phi^2} \rho \delta, \quad (12.48)$$

which can be regarded as the mode induced by the matter perturbation $\delta\rho$. In general there exists an oscillating mode of the field perturbation, but it is neglected relative to the matter-induced mode under the quasi-static approximation.

The gravitational potential Ψ can be expressed in terms of δ as

$$\frac{k^2}{a^2} \Psi \simeq -4\pi G_{\text{eff}} \rho \delta, \quad (12.49)$$

where G_{eff} is the effective gravitational coupling given by

$$\begin{aligned} G_{\text{eff}} &= \frac{2M_{\text{pl}}^2[(B_6 D_9 - B_7^2)(k/a)^2 - B_6 M_\phi^2]}{(A_6^2 B_6 + B_8^2 D_9 - 2A_6 B_7 B_8)(k/a)^2 - B_8^2 M_\phi^2} G \\ &= \frac{2M_{\text{pl}}^2[2H^2 w_1^2 + 2\dot{w}_1(\dot{w}_1 + 2Hw_1) - w_4(\dot{w}_2 + Hw_2) - w_4\rho + w_4\dot{\phi}^2(M_\phi a/k)^2]}{2Hw_1^2 w_2 - w_2^2 w_4 + 4w_1 w_2 \dot{w}_1 - 2w_1^2 \dot{w}_2 - 2w_1^2 \rho + 2w_1^2 \dot{\phi}^2(M_\phi a/k)^2} G. \end{aligned} \quad (12.50)$$

Here we have introduced the Newton gravitational constant $G = (8\pi M_{\text{pl}}^2)^{-1}$ for the comparison with G_{eff} .

From Eq. (12.30) the term $\dot{\mathcal{V}} \sim H\mathcal{V}$ is at most of the order of Ψ , so the terms on the right hand side of Eq. (12.31) can be neglected relative to the left hand side of it. From Eq. (12.29) the term $H\mathcal{V}$ is at most of the order of $(aH/k)^2 \delta \ll \delta$ for $k \gg aH$, so that $\delta_m \simeq \delta$ in Eq. (12.28). Then, the matter perturbation Eq. (12.31) approximately reduces to

$$\ddot{\delta}_m + 2H\dot{\delta}_m - 4\pi G_{\text{eff}} \rho \delta_m \simeq 0. \quad (12.51)$$

Thus, the growth rate of matter perturbations is affected by the modification of the effective gravitational coupling G_{eff} . In Sec. 12.4, we will compute G_{eff} in concrete modified gravity models of dark energy.

We define the gravitational slip parameter $\eta \equiv -\Phi/\Psi$ to characterize the difference between the two Bardeen potentials $-\Psi$ and Φ . From Eqs. (12.45)–(12.47) it follows that

$$\eta \simeq \frac{(B_8 D_9 - A_6 B_7)(k/a)^2 - B_8 M_\phi^2}{(B_6 D_9 - B_7^2)(k/a)^2 - B_6 M_\phi^2}. \quad (12.52)$$

As we showed in Sec. 8.7, the effective gravitational potential related to the deviation of light rays in weak lensing and CMB observations is given by $\psi_{\text{eff}} = \Phi - \Psi$. From

Eq. (12.49) this obeys [19, 24, 25]

$$\psi_{\text{eff}} \simeq 8\pi G_{\text{eff}} \frac{1+\eta}{2} \left(\frac{a}{k}\right)^2 \rho \delta_m. \quad (12.53)$$

In GR with the functions $G_2 = K(\phi, X)$, $G_3 = 0$, $G_4 = M_{\text{pl}}^2/2$, $G_5 = 0$, we have $B_6 = B_8 = 2M_{\text{pl}}^2$ and $A_6 = B_7 = 0$, in which case $G_{\text{eff}} = G$ and $\eta = 1$. Then, the solution to Eq. (12.51) during the matter dominance ($3H^2 \simeq 8\pi G\rho$ and $\dot{H}/H^2 \simeq -3/2$) is given by $\delta_m \propto a$, under which $\psi_{\text{eff}} \simeq \text{constant}$. In modified gravity theories, both δ_m and ψ_{eff} generally differ from those in GR. In Sec. 12.4, we will discuss constraints on several concrete models from the cosmic growth history.

12.3. Second-order actions for cosmological perturbations in Horndeski theories

The alternative prescription for the derivation of the linear perturbation equations of motion in Horndeski theories is to expand the action (12.13) up to second order in perturbations. By doing this, it is possible to identify conditions for avoiding ghosts and Laplacian instabilities of scalar and tensor perturbations. We do not consider vector perturbations as they do not give rise to additional conditions to those derived for scalar and tensor modes in Horndeski theories. We begin with the perturbed metric given by

$$ds^2 = -(1 + 2\Psi) dt^2 + 2\chi_{|i} dt dx^i + a^2(t) [(1 + 2\Phi)\delta_{ij} + h_{ij}] dx^i dx^j, \quad (12.54)$$

where Ψ, χ, Φ are scalar perturbations and h_{ij} is the tensor perturbation obeying the traceless and transverse conditions. We choose the unitary gauge under which the scalar-field perturbation $\delta\phi$ vanishes, i.e.,

$$\delta\phi = 0. \quad (12.55)$$

The theoretically consistent conditions derived in this section are not affected by gauge choices.

As for the matter sector, we take into account two perfect fluids labelled by $i = r, m$ (which correspond to radiation and non-relativistic matter, respectively). We denote the density and the pressure of fluids as ρ_i and P_i for the background, respectively, with the equations of state satisfying $w_i = P_i/\rho_i \geq 0$. We also introduce the matter perturbation $\delta\rho_i$ as well as the velocity potential $\mathcal{V}_i = -\delta q_i/(\rho_i + P_i)$.

First, we expand the action (12.13) up to second order in tensor perturbations. In doing so, we write h_{ij} as Eq. (6.153) with the two polarization tensors e_{ij}^+ and $e_{ij}^\times$ obeying the normalizations (6.154). Following the similar procedure to that explained in Sec. 6.7.3, the resulting second-order action of tensor perturbations (derived after integrations by parts) is

$$S_t^{(2)} = \sum_{\lambda=+, \times} \int dt d^3x a^3 Q_t \left[\dot{h}_\lambda^2 - \frac{c_t^2}{a^2} (\partial h_\lambda)^2 \right], \quad (12.56)$$

where

$$Q_t = \frac{w_1}{4}, \quad c_t^2 = \frac{w_4}{w_1}. \quad (12.57)$$

The quantities w_1 and w_4 are defined, respectively, by Eqs. (12.32) and (12.35). In Fourier space, the variation of the action (12.56) with respect to h_λ gives the equation of motion

$$\ddot{h}_\lambda + \left(3H + \frac{\dot{Q}_t}{Q_t}\right) \dot{h}_\lambda + c_t^2 \frac{k^2}{a^2} h_\lambda = 0. \quad (12.58)$$

To avoid the ghost and the Laplacian instabilities of tensor perturbations, we require that

$$Q_t > 0, \quad (12.59)$$

$$c_t^2 > 0, \quad (12.60)$$

which are satisfied for $w_1 > 0$ and $w_4 > 0$.

For scalar perturbations, we consider the Horndeski action (12.1) in the presence of the Schutz–Sorkin action with two matter fluids (radiation and non-relativistic matter), i.e.,

$$S = S^H - \int d^4x \sum_{i=r,m} [\sqrt{-g} \rho_i(n) + J_i^\mu \partial_\mu \ell_i], \quad (12.61)$$

where the definitions of J_i^μ and ℓ_i are given in Sec. 6.9. The density perturbations $\delta\rho_i$ and the velocity potentials $\mathcal{V}_i$ obey the same equations of motion as Eqs. (6.227) and (6.228). The latter equations are

$$\dot{\mathcal{V}}_i - \Psi - 3H c_i^2 \mathcal{V}_i - \frac{c_i^2}{\rho_i + P_i} \delta\rho_i = 0, \quad (12.62)$$

where c_i 's ($i = r, m$) are the propagation speeds of two fluids.

We expand the action (12.61) up to second order in scalar perturbations and employ Eq. (12.62) to eliminate the $\delta\rho_i$ term. Then, the second-order action of scalar perturbations yields

$$\begin{aligned} S_s^{(2)} = & \int dt d^3x a^3 \left[(2w_1 \dot{\Phi} - w_2 \Psi) \frac{\nabla^2 \chi}{a^2} + \frac{w_3}{3} \Psi^2 + \frac{w_4}{a^2} (\partial\Phi)^2 - 3w_1 \dot{\Phi}^2 \right. \\ & \left. + \left(3w_2 \dot{\Phi} - 2w_1 \frac{\nabla^2 \Phi}{a^2} \right) \Psi \right] + S_M^{(2)}, \end{aligned} \quad (12.63)$$

where w_2 and w_3 are given, respectively, by Eqs. (12.33) and (12.34), and

$$\begin{aligned} \mathcal{S}_M^{(2)} = \sum_{i=r,m} \int dt d^3x a^3 (\rho_i + P_i) & \left[\frac{\dot{\mathcal{V}}_i^2}{2c_i^2} - \frac{(\partial \mathcal{V}_i)^2}{2a^2} + \frac{3}{2} \dot{H} \mathcal{V}_i^2 - \frac{1}{a^2} \partial \mathcal{V}_i \partial \chi \right. \\ & \left. + \left(\dot{\mathcal{V}}_i - 3H c_i^2 \mathcal{V}_i \right) \left(3\Phi - \frac{\Psi}{c_i^2} \right) + \frac{\Psi^2}{2c_i^2} \right]. \end{aligned} \quad (12.64)$$

The matter action $\mathcal{S}_M^{(2)}$ is the extension of Eq. (6.230) to the case of two fluids.

Varying the action (12.63) with respect to χ , it follows that

$$w_2 \Psi = 2w_1 \dot{\Phi} + \sum_{i=r,m} (\rho_i + P_i) \mathcal{V}_i. \quad (12.65)$$

Substituting the relation (12.65) into Eq. (12.64) to eliminate Ψ , the terms containing the derivatives of χ cancel each other. Then, we are left with the three dynamical degrees of freedom $\Phi, \mathcal{V}_r, \mathcal{V}_m$. Integrating the terms $\dot{\Phi} \partial^2 \Phi$ and $\mathcal{V}_i \partial^2 \Phi$ by parts, the second-order action of scalar perturbations can be expressed in the form

$$S_s^{(2)} = \int dt d^3x a^3 \left(\dot{\vec{\mathcal{X}}}^t \mathbf{K} \vec{\mathcal{X}} - \partial_j \vec{\mathcal{X}}^t \mathbf{G} \partial^j \vec{\mathcal{X}} - \vec{\mathcal{X}}^t \mathbf{M} \vec{\mathcal{X}} - \vec{\mathcal{X}}^t \mathbf{B} \dot{\vec{\mathcal{X}}} \right), \quad (12.66)$$

where $\mathbf{K}, \mathbf{G}, \mathbf{M}, \mathbf{B}$ are 3×3 matrices, and the vector field $\vec{\mathcal{X}}$ is defined by

$$\vec{\mathcal{X}}^t = (\Phi, \mathcal{V}_r, \mathcal{V}_m). \quad (12.67)$$

The matrix $\mathbf{M}$ is related to the masses of scalar modes. In the following, we focus on the behavior of perturbations in the small-scale limit, in which case the second term on the right hand side of Eq. (12.66) dominates over the third and the fourth terms.

Provided that the symmetric matrix $\mathbf{K}$ is positive definite, the scalar ghosts are absent. The positivity of $\mathbf{K}$ is guaranteed under the following conditions

$$Q_s \equiv \frac{w_1(4w_1w_3 + 9w_2^2)}{3w_2^2} > 0, \quad (12.68)$$

$$\rho_i + P_i > 0, \quad (i = r, m). \quad (12.69)$$

The conditions (12.69) are satisfied for radiation and non-relativistic matter.

In Fourier space with the coming wavenumber k and the frequency ω , the non-vanishing solution to $\vec{\mathcal{X}}$ exists under the condition

$$\det \left(\omega^2 \mathbf{K} - \frac{k^2}{a^2} \mathbf{G} \right) = 0, \quad (12.70)$$

where we ignored the third and fourth terms of Eq. (12.66) in the small-scale limit. We define the scalar propagation speed c_S according to the relation $\omega^2 = c_S^2 k^2 / a^2$. Then, there are three solutions to c_S^2 . Two of them are the radiation and matter propagation speed squares c_r^2 and c_m^2 . For perfect fluids, they are equivalent to the equations of state $w_r = 1/3$ and $w_m = 0^+$, respectively, so there are no Laplacian

instabilities for the matter sector. Another is the propagation speed squared of the perturbation Φ , which is given by

$$c_s^2 = \frac{3(2Hw_1^2w_2 - w_2^2w_4 + 4w_1w_2\dot{w}_1 - 2w_1^2\dot{w}_2) - 6w_1^2\sum_i(\rho_i + P_i)}{w_1(4w_1w_3 + 9w_2^2)}. \quad (12.71)$$

To avoid the Laplacian instability, we require that

$$c_s^2 > 0. \quad (12.72)$$

From Eq. (12.71), the scalar sound speed c_s is affected by the existence of matter fluids. After the above diagonalization, the equation of motion of Φ contains the Laplacian term $c_s^2 k^2/a^2$. The quasi-static approximation employed in Sec. 12.2 for deriving G_{eff} and η is valid for the physical wavenumber deep inside the sound horizon ($a/k \ll c_s H^{-1}$, i.e., $c_s k/a \gg H$).

The above discussion shows that Horndeski theories need to satisfy the four conditions (12.59), (12.60), (12.68), and (12.72) for theoretical consistency. In the rest of this section, we will express G_{eff} and η by using the variables Q_t, c_t^2, Q_s, c_s^2 . In doing so, we take into account non-relativistic matter alone (energy density ρ) by neglecting the contribution of radiation, such that $\sum_i(\rho_i + P_i) = \rho$. From Eq. (12.57), we have $w_1 = 4Q_t$ and $w_4 = c_t^2 w_1$. From (12.68) and (12.71), the terms w_3 and ρ can be expressed in terms of Q_s and c_s^2 . Then, we can write Eqs. (12.50) and (12.52) in the following forms [26, 27]

$$G_{\text{eff}} = \frac{c_t^2 M_{\text{pl}}^2}{4Q_t} \left[1 + \frac{4Q_t \mathcal{B}^2}{c_t^2 \mathcal{A}(k)} \right] G, \quad (12.73)$$

$$\eta = \frac{\mathcal{A}(k) + 4Q_t \mathcal{B}\mathcal{C}}{\mathcal{A}(k)c_t^2 + 4Q_t \mathcal{B}^2}, \quad (12.74)$$

where

$$\mathcal{A}(k) = Q_s c_s^2 w_2^2 + 32Q_t^2 \dot{\phi}^2 \left(\frac{M_\phi a}{k} \right)^2, \quad (12.75)$$

$$\mathcal{B} = 8\dot{Q}_t + 8H Q_t - c_t^2 w_2, \quad (12.76)$$

$$\mathcal{C} = 8H Q_t - w_2. \quad (12.77)$$

From Eq. (12.53), the effective gravitational potential $\psi_{\text{eff}} = \Phi - \Psi$ obeys

$$\psi_{\text{eff}} \simeq 8\pi G \mathcal{F} \left(\frac{a}{k} \right)^2 \rho \delta_m, \quad (12.78)$$

where the quantity $\mathcal{F}$, which is defined by $\mathcal{F} \equiv (G_{\text{eff}}/G)(1+\eta)/2$, can be expressed as

$$\mathcal{F} = \frac{(1 + c_t^2)M_{\text{pl}}^2}{8Q_t} + \frac{\mathcal{B}(\mathcal{B} + \mathcal{C})M_{\text{pl}}^2}{2\mathcal{A}(k)}. \quad (12.79)$$

GR corresponds to $Q_t = M_{\text{pl}}^2/4$, $c_t^2 = 1$, $w_2 = 2HM_{\text{pl}}^2$, $\mathcal{B} = 0$, $\mathcal{C} = 0$, and hence $G_{\text{eff}} = G$, $\eta = 1$, $\mathcal{F} = 1$.

The term $c_t^2 M_{\text{pl}}^2/(4Q_t)$ in G_{eff} , which is associated with tensor perturbations, is positive under the two conditions (12.59) and (12.60). The term $4Q_t \mathcal{B}^2/(c_t^2 \mathcal{A}(k))$ is also positive under the four conditions (12.59), (12.60), (12.68) and (12.72). The latter corresponds to the interaction between the scalar degree of freedom and the matter sector. As long as the ghost and the Laplacian instabilities are absent, the scalar-matter interaction enhances the gravitational attraction with matter.

If the condition $c_t^2 M_{\text{pl}}^2/(4Q_t) > 1$ is satisfied, then G_{eff} is always larger than G under the theoretically consistent conditions. If we want to realize G_{eff} smaller than G , the *necessary* condition is given by $c_t^2 M_{\text{pl}}^2/(4Q_t) < 1$ [27]. However, due to the existence of the positive term $4Q_t \mathcal{B}^2/(c_t^2 \mathcal{A}(k))$, this is not a sufficient condition for realizing $G_{\text{eff}} < G$. Even when $c_t^2 M_{\text{pl}}^2/(4Q_t) < 1$, there are models like covariant Galileons in which the term $4Q_t \mathcal{B}^2/(c_t^2 \mathcal{A}(k))$ leads to G_{eff} larger than G [28].

If the mass term M_ϕ is sufficiently large such that the condition $M_\phi \gg k/a$ is satisfied, we can take the limit $\mathcal{A}(k) \rightarrow \infty$ in Eqs. (12.73) and (12.74), such that

$$G_{\text{eff}} \rightarrow \frac{c_t^2 M_{\text{pl}}^2}{4Q_t} G, \quad (12.80)$$

$$\eta \rightarrow \frac{1}{c_t^2}, \quad (12.81)$$

which are expressed in terms of the quantities associated with tensor perturbations alone. In another massless limit ($M_\phi \ll k/a$), we have $\mathcal{A}(k) \rightarrow Q_s c_s^2 w_2^2$ and hence

$$G_{\text{eff}} \rightarrow \frac{c_t^2 M_{\text{pl}}^2}{4Q_t} \left(1 + \frac{4Q_t \mathcal{B}^2}{Q_s c_s^2 w_2^2} \right) G, \quad (12.82)$$

$$\eta \rightarrow \frac{Q_s c_s^2 w_2^2 + 4Q_t \mathcal{B}^2}{Q_s c_s^2 w_2^2 + 4Q_t \mathcal{B}^2}, \quad (12.83)$$

where k -dependence is not present. In this massless regime, the scalar-matter interaction provides the important contributions to G_{eff} and η .

There are modified gravity models like those based on $f(R)$ gravity in which the mass M_ϕ is large in the early cosmological epoch and it decreases to give rise to the late-time cosmic acceleration. In such cases, the transition from the regime $M_\phi \gg k/a$ to $M_\phi \ll k/a$ occurs by today. Meanwhile, there are models like covariant Galileons in which the scalar field is nearly massless such that G_{eff} and η are given, respectively, by (12.82) and (12.83). In both cases the large-distance modification of gravity arises in the massless regime ($M_\phi \ll k/a$).

12.4. Constraints on dark energy models in the framework of Horndeski theories

Since we have derived the linear perturbation equations and theoretically consistent conditions in a general way, we now apply them to concrete modified gravity models in the framework of Horndeski theories, e.g., $f(R)$ gravity, Brans–Dicke theories,

and covariant Galileons. This is important to distinguish the models from the observations of galaxy clusterings, redshift-space distortions, CMB and weak lensing. Since we are interested in the evolution of matter perturbations after the end of the radiation era, we take into account non-relativistic matter alone. Throughout this section, we take the Newtonian gauge $\chi = 0$ in the perturbed metric (12.54).

12.4.1. $f(R)$ gravity

Let us first discuss $f(R)$ gravity with the action (11.1). As we showed in Sec. 11.2.1, metric $f(R)$ gravity is equivalent to BD theory given by the action (11.77) with the BD parameter $\omega_{\text{BD}} = 0$. In the action (11.77), the dimensionless field χ corresponds to the quantity $f_{,R}$ with the potential $V = (M_{\text{pl}}^2/2)(Rf_{,R} - f)$. We redefine the scalar field ϕ (having a dimension of mass) as $\phi \equiv M_{\text{pl}}\chi = M_{\text{pl}}f_{,R}$. In the Language of Horndeski theories, the action (11.77) corresponds to the functions

$$G_2 = -\frac{M_{\text{pl}}^2}{2}(Rf_{,R} - f), \quad G_4 = \frac{1}{2}M_{\text{pl}}\phi, \quad G_3 = 0 = G_5. \quad (12.84)$$

From Eqs. (12.19), (12.20) and (12.22), we obtain the background equations of motion

$$G_2 + 3M_{\text{pl}}H^2\phi + 3M_{\text{pl}}H\dot{\phi} = \rho, \quad (12.85)$$

$$2M_{\text{pl}}\phi\dot{H} + M_{\text{pl}}\ddot{\phi} - M_{\text{pl}}H\dot{\phi} = -\rho - P, \quad (12.86)$$

$$G_{2,\phi} = -3(2H^2 + \dot{H})M_{\text{pl}}, \quad (12.87)$$

where we have not omitted the pressure P . On using the continuity equation (12.21), the field equation (12.87) follows from Eqs. (12.85) and (12.86). We recover Eqs. (11.18) and (11.19) by substituting $G_2 = -(M_{\text{pl}}^2/2)(Rf_{,R} - f)$, $\phi = f_{,R}M_{\text{pl}}$, $\rho = \rho_m$, and $P = 0$ into Eqs. (12.85) and (12.86).

The variables (12.32)–(12.35) are given, respectively, by $w_1 = M_{\text{pl}}\phi$, $w_2 = M_{\text{pl}}(\dot{\phi} + 2H\phi)$, $w_3 = -9HM_{\text{pl}}(\dot{\phi} + H\phi)$, and $w_4 = M_{\text{pl}}\phi$. The quantities Q_t and c_t^2 in Eq. (12.57) yield

$$Q_t = \frac{1}{4}M_{\text{pl}}\phi, \quad c_t^2 = 1. \quad (12.88)$$

On using the background equation (12.86), the quantities Q_s and c_s^2 defined by Eqs. (12.68) and (12.71) reduce, respectively, to

$$Q_s = \frac{3M_{\text{pl}}\dot{\phi}^2\phi}{(\dot{\phi} + 2H\phi)^2}, \quad c_s^2 = 1. \quad (12.89)$$

Hence the tensor and scalar ghosts are absent under the condition

$$\phi = M_{\text{pl}}f_{,R} > 0, \quad (12.90)$$

which corresponds to Eq. (11.11). Since both c_t^2 and c_s^2 are equivalent to the speed of light, there are no Laplacian instabilities of small-scale perturbations.

Since the quantities (12.75)–(12.77) are given, respectively, by $\mathcal{A}(k) = M_{\text{pl}}^2 \dot{\phi}^2 \phi [3M_{\text{pl}} + 2\phi(M_\phi a/k)^2]$, $\mathcal{B} = M_{\text{pl}} \dot{\phi}$, and $\mathcal{C} = -M_{\text{pl}} \dot{\phi}$, the effective gravitational coupling (12.73), the gravitational slip parameter (12.74), and the quantity (12.79) reduce, respectively, to [19]

$$G_{\text{eff}} = \frac{M_{\text{pl}}}{\phi} \frac{4 + 2(\phi/M_{\text{pl}})(M_\phi a/k)^2}{3 + 2(\phi/M_{\text{pl}})(M_\phi a/k)^2} G, \quad (12.91)$$

$$\eta = \frac{1 + (\phi/M_{\text{pl}})(M_\phi a/k)^2}{2 + (\phi/M_{\text{pl}})(M_\phi a/k)^2}, \quad (12.92)$$

$$\mathcal{F} = \frac{M_{\text{pl}}}{\phi} = \frac{1}{f_{,R}}. \quad (12.93)$$

From Eq. (B.1) in Appendix B, the mass squared M_ϕ^2 reads $M_\phi^2 = -G_{2,\phi\phi}$. Since the quantity $G_2 = -(M_{\text{pl}}^2/2)(Rf_{,R} - f)$ depends on ϕ through the relation $\phi = M_{\text{pl}} f_{,R}$, we have $G_{2,\phi} = -M_{\text{pl}} R/2$, $G_{2,\phi\phi} = -1/(2f_{,RR})$, and hence

$$M_\phi^2 = \frac{1}{2f_{,RR}} = \frac{R}{2mf_{,R}}, \quad (12.94)$$

where $m = Rf_{,RR}/f_{,R}$ is the deviation parameter from the Λ CDM model introduced in Sec. 11.1. Then, we can write Eqs. (12.91) and (12.93) in the forms [18]

$$G_{\text{eff}} = \frac{1 + 4(f_{,RR}/f_{,R})(k/a)^2}{1 + 3(f_{,RR}/f_{,R})(k/a)^2} \frac{G}{f_{,R}}, \quad \eta = \frac{1 + 2(f_{,RR}/f_{,R})(k/a)^2}{1 + 4(f_{,RR}/f_{,R})(k/a)^2}, \quad (12.95)$$

respectively.

As we already discussed in Sec. 11.1, the viable $f(R)$ dark energy models (11.14)–(11.16) are close to the Λ CDM model in the early Universe ($R \gg R_0$). In this regime, the parameter m is much smaller than 1 with $f_{,R} \simeq 1$, so that $M_\phi^2 \gg R$ from Eq. (12.94). The deviation from the Λ CDM model arises at the late cosmological epoch with the increase of m . The quantity $f_{,R}$ also starts to deviate from 1, but it is of the order of 1 today for viable $f(R)$ models. If the parameter m grows to the value of the order of 0.1 by today, the mass M_ϕ can decrease to the order of H_0 .

Since M_ϕ decreases quite rapidly from the past to today, we expect that there is a transition from the “massive” regime $M_\phi^2 > k^2/a^2$ to the “massless” regime $M_\phi^2 < k^2/a^2$. The moment of the transition depends on the wavenumber k . The wavenumber related to the linear region of the observed galaxy power spectrum is given by [29]

$$0.01 \, h \, \text{Mpc}^{-1} \lesssim k \lesssim 0.2 \, h \, \text{Mpc}^{-1}. \quad (12.96)$$

The region (12.96) corresponds to $30a_0H_0 \lesssim k \lesssim 600a_0H_0$. Provided that M_ϕ decreases to the order close to H_0 by today, the transition from the regime

$M_\phi^2 > k^2/a^2$ to the regime $M_\phi^2 < k^2/a^2$ occurred in the past. For larger k , earlier the moment of the transition is. Taking $k = 600a_0H_0$ as the largest wavenumber for linear perturbations, the condition for entering the regime $M_\phi^2 < k^2/a^2$ by today (the redshift $z = 0$) is given by [30]

$$m(z=0) \gtrsim 10^{-5}, \quad (12.97)$$

where we used the approximations $f_{,R} \approx 1$ and $R(z=0) \approx 10H_0^2$.

From Eqs. (12.91) and (12.93), we have that $G_{\text{eff}} \simeq (M_{\text{pl}}/\phi)G$ and $\eta \simeq 1$ for $M_\phi^2 \gg k^2/a^2$ and that $G_{\text{eff}} \simeq (4/3)(M_{\text{pl}}/\phi)G$ and $\eta \simeq 1/2$ for $M_\phi^2 \ll k^2/a^2$. Hence the gravitational interaction with matter is enhanced in the latter regime. Under the quasi-static approximation on sub-horizon scales, the gauge-invariant matter density contrast δ_m obeys Eq. (12.51) with G_{eff} given by Eq. (12.91). On using $\mathcal{N} = \ln a$ and $w_{\text{eff}} = -1 - 2\dot{H}/(3H^2)$, we can write Eq. (12.51) in the form

$$\frac{d^2\delta_m}{d\mathcal{N}^2} + \left(\frac{1}{2} - \frac{3}{2}w_{\text{eff}}\right) \frac{d\delta_m}{d\mathcal{N}} - \frac{3}{2}\Omega_m \frac{4 + 2f_{,R}(M_\phi a/k)^2}{3 + 2f_{,R}(M_\phi a/k)^2} \delta_m \simeq 0, \quad (12.98)$$

where $\Omega_m = 8\pi G\rho/(3f_{,R}H^2)$. On using Eqs. (12.78) and (12.93), the effective gravitational potential obeys

$$\psi_{\text{eff}} \simeq 3 \left(\frac{aH}{k}\right)^2 \Omega_m \delta_m. \quad (12.99)$$

The matter-dominated epoch corresponds to $w_{\text{eff}} \simeq 0$ and $\Omega_m \simeq 1$. In the regime $M_\phi^2 \gg k^2/a^2$, the growing-mode solution to Eq. (12.98) during the matter dominance is given by

$$\delta_m \propto t^{2/3}, \quad (12.100)$$

which mimics the evolution of GR. From Eqs. (12.99) and (12.100), it follows that $\psi_{\text{eff}} = \text{constant}$. In another regime $M_\phi^2 \ll k^2/a^2$, the evolution of δ_m during the matter era is modified to [21, 22]

$$\delta_m \propto t^{(\sqrt{33}-1)/6}, \quad (12.101)$$

whose growth rate is larger than Eq. (12.100). In this region, the effective gravitational potential evolves as

$$\psi_{\text{eff}} \propto t^{(\sqrt{33}-5)/6}, \quad (12.102)$$

which grows in time. After the Universe enters the epoch of cosmic acceleration, the growth rates of δ_m and ψ_{eff} get smaller than those given by Eqs. (12.101) and (12.102), respectively.

We caution that the above analytic solutions have been derived under the quasi-static approximation for the modes deep inside the Hubble radius ($k \gg aH$). By doing this, we have neglected the oscillating mode of the field perturbation $\delta\phi = M_{\text{pl}}\delta f_{,R}$ relative to the mode induced by matter perturbations. To see the

validity of this approximation, we need to solve full perturbation equations of motion numerically. From Eqs. (12.36), (12.37), (12.39) and (12.43), we obtain the following three independent equations in the Newtonian gauge ($\chi = 0$):

$$\ddot{\delta\phi} + 3H\dot{\delta\phi} + \left(\frac{k^2}{a^2} + M^2\right)\delta\phi = \frac{\delta\rho}{3M_{\text{pl}}} + 2\ddot{\phi}\Psi + \dot{\phi}\left(\dot{\Psi} - 3\dot{\Phi} + 6H\Psi\right), \quad (12.103)$$

$$\begin{aligned} \frac{k^2}{a^2}\Phi + 3H\left(\dot{\Phi} - H\Psi\right) - \frac{1}{2\dot{\phi}}\left[\left(3H^2 + 3\dot{H} - \frac{k^2}{a^2}\right)\delta\phi - 3H\dot{\delta\phi} \right. \\ \left. + 3\dot{\phi}\left(2H\Psi - \dot{\Phi}\right) + \frac{\delta\rho}{M_{\text{pl}}}\right] = 0, \end{aligned} \quad (12.104)$$

$$\Psi + \Phi = -\frac{\delta\phi}{\dot{\phi}}, \quad (12.105)$$

where

$$M^2 \equiv \frac{2\phi}{3M_{\text{pl}}}M_\phi^2 - \frac{R}{3} = \frac{1}{3}\left(\frac{f_{,R}}{f_{,RR}} - R\right). \quad (12.106)$$

From Eq. (12.103), the quantity M can be identified as a mass term of the field perturbation $\delta\phi$. As we already mentioned in Sec. 11.1, we require the condition $f_{,RR} > 0$ to avoid the tachyonic growth of the field perturbation $\delta\phi$ in the early cosmological epoch.

The density contrast $\delta = \delta\rho/\rho$ and the velocity potential $\mathcal{V}$ obey Eqs. (12.29) and (12.30), respectively, so the evolution of $\delta\phi, \Phi, \Psi, \delta, \mathcal{V}$ is determined by numerically integrating Eqs. (12.103)–(12.105), (12.29) and (12.30) with $\chi = 0$ for a given $f(R)$ model. In doing so, we need to provide initial conditions of these variables. In particular, the field perturbation $\delta\phi$ obeys the second-order differential equation (12.103), so it is necessary to give the initial conditions of $\delta\phi$ and $\dot{\delta\phi}$. Since the mass M is large in the early matter era for viable $f(R)$ dark energy models, the rapid oscillation of $\delta\phi$ may be induced depending on its initial conditions.

To study the evolution of $\delta\phi$, we focus on the sub-horizon perturbations and neglect terms containing the gravitational potentials Ψ and Φ in Eq. (12.103). This approximation gives

$$\ddot{\delta\phi} + 3H\dot{\delta\phi} + \left(\frac{k^2}{a^2} + M^2\right)\delta\phi \simeq \frac{\delta\rho}{3M_{\text{pl}}}. \quad (12.107)$$

The special solution to this equation is the perturbation $\delta\phi_{\text{ind}}$ induced by the matter perturbation $\delta\rho$, i.e.,

$$\delta\phi_{\text{ind}} \simeq \frac{\delta\rho}{3M_{\text{pl}}(k^2/a^2 + M^2)}, \quad (12.108)$$

which corresponds to Eq. (12.48) derived under the quasi-static approximation. The general solution to Eq. (12.107) is the sum of the special solution (12.108) and the

oscillating mode $\delta\phi_{\text{osc}}$ obeying the differential equation

$$\ddot{\delta\phi}_{\text{osc}} + 3H\dot{\delta\phi}_{\text{osc}} + \left(\frac{k^2}{a^2} + M^2\right)\delta\phi_{\text{osc}} = 0. \quad (12.109)$$

Provided that the frequency $\omega = \sqrt{k^2/a^2 + M^2}$ satisfies the adiabatic condition $|\dot{\omega}| \ll \omega^2$, the WKB approximation allows us to derive the solution to Eq. (12.109) in the form

$$\delta\phi_{\text{osc}} \simeq \frac{\beta}{a^{3/2}\sqrt{2\omega}} \cos\left(\int \omega dt\right), \quad (12.110)$$

where β is a constant. The general solution to Eq. (12.107) is given by $\delta\phi = M_{\text{pl}}f_{,RR}\delta R = \delta\phi_{\text{ind}} + \delta\phi_{\text{osc}}$, so the perturbation in the Ricci scalar reads

$$\delta R \simeq \frac{1}{3f_{,RR}} \frac{\delta\rho}{M_{\text{pl}}^2(k^2/a^2 + M^2)} + \frac{\beta}{f_{,RR}M_{\text{pl}}a^{3/2}\sqrt{2\omega}} \cos\left(\int \omega dt\right). \quad (12.111)$$

The second term on the right hand side of Eq. (12.111), which we denote δR_{osc} , induces the oscillation of R .

During the matter dominance, the scale factor a and the background Ricci scalar $R^{(0)}$ evolve as $a \propto t^{2/3}$ and $R^{(0)} \propto t^{-2}$, respectively. The relative amplitude of δR_{osc} to $R^{(0)}$ has the dependence

$$\frac{|\delta R_{\text{osc}}|}{R^{(0)}} \propto \frac{t}{f_{,RR}(k^2/a^2 + M^2)^{1/4}}. \quad (12.112)$$

For concreteness, let us consider the $f(R)$ models (11.14) and (11.15). On using the asymptotic form (11.17) for $R \gg R_0$, the mass squared $M^2 \simeq 1/(3f_{,RR})$ evolves as $M^2 \propto R^{2(n+1)} \propto t^{-4(n+1)}$ during the matter era. In the regime $M^2 \gg k^2/a^2$, we have $|\delta R_{\text{osc}}|/R^{(0)} \propto t^{-(3n+2)}$ and hence the amplitude of the oscillating mode decreases faster than $R^{(0)}$.

As we go back to the past, the contribution of the oscillating mode to the Ricci scalar R tends to be more important. This property persists in the radiation era as well [21]. To avoid the negative value of R induced by the oscillating mode δR_{osc} , we require that δR_{osc} is smaller than $R^{(0)}$ in the early cosmological epoch. If R crosses 0, the theoretically consistent conditions like $f_{,R} > 0$ and $f_{,RR} > 0$ tend to be violated. In other words, we need to fine-tune initial conditions of δR such that the oscillating mode δR_{osc} is suppressed relative to the matter-induced mode δR_{ind} , i.e, the first term on the right hand side of Eq. (12.111). Otherwise the system can access a curvature singularity [31].

As long as the condition $|\delta R_{\text{osc}}| \ll |\delta R_{\text{ind}}|$ is initially satisfied, the dominant contribution to δR comes from the matter-induced mode δR_{ind} . In this case the quasi-static approximation should be trustable, so the evolution of δ_m and ψ_{eff} can be described by Eqs. (12.98) and (12.99). In fact, the numerical integration of full perturbation equations of motion shows that this is indeed the case [30, 32]. We can

resort to the approximate equations (12.98) and (12.99) to study the evolution of perturbations after the onset of the matter era.

On using the asymptotic form (11.17) of the models (11.14) and (11.15), we can estimate the transition redshift z_k at which M_ϕ^2 becomes equivalent to k^2/a^2 . In doing so, we assume that the transition occurs in the early matter era satisfying $z_k > \mathcal{O}(1)$. During the matter dominance, we use the approximations $H^2 \simeq H_0^2 \Omega_m^{(0)} (1+z)^3$ and $R \simeq 3H^2$. Today's dark energy density is approximately given by $\rho_{\text{DE}}^{(0)} \approx \lambda M_{\text{pl}}^2 R_0/2$, so that $\lambda R_0 \approx 6H_0^2 \Omega_{\text{DE}}^{(0)}$. Then, the transition redshift can be estimated as

$$z_k = \left[\left(\frac{k}{a_0 H_0} \right)^2 \frac{4n(2n+1)}{3\lambda^{2n}} \frac{(2\Omega_{\text{DE}}^{(0)})^{2n+1}}{(\Omega_m^0)^{2(n+1)}} \right]^{1/(6n+4)} - 1. \quad (12.113)$$

For $n = 1$, $\lambda = 3$, $\Omega_m^{(0)} = 0.32$, $k = 300a_0 H_0$, we have $z_k = 4.0$.

For larger k , the transition occurs at higher redshifts. The time t_k at the transition is related to z_k as $z_k + 1 = a_0/a_k \propto t_k^{-2/3}$, so it has the k -dependence $t_k \propto k^{-3/(6n+4)}$. For $t > t_k$, the matter density contrast evolves as $\delta_m \propto t^{(\sqrt{33}-1)/6}$ by the time $t = t_{\text{DE}}$ at which the cosmic acceleration sets in ($\ddot{a} = 0$). The matter power spectrum $P_{\delta_m} \propto |\delta_m|^2$ at the time t_{DE} shows the difference compared to the case of the Λ CDM model, as [21]

$$\frac{P_{\delta_m}(t_{\text{DE}})}{P_{\delta_m}^{\Lambda\text{CDM}}(t_{\text{DE}})} = \left(\frac{t_{\text{DE}}}{t_k} \right)^{2\left(\frac{\sqrt{33}-1}{6} - \frac{2}{3}\right)} \propto k^{\Delta n_s}, \quad (12.114)$$

where

$$\Delta n_s = \frac{\sqrt{33} - 5}{2(3n + 2)}. \quad (12.115)$$

Today's ratio of the two power spectra, i.e., $P_{\delta_m}(t_0)/P_{\delta_m}^{\Lambda\text{CDM}}(t_0)$, is generally different from Eq. (12.114), but the numerical simulation shows that the difference is small for n of the order of unity [22].

The estimation (12.114) shows that the $f(R)$ models (11.14) and (11.15) can be distinguished from the Λ CDM model from the observations of the matter power spectrum. The modified evolution (12.102) of ψ_{eff} at low redshifts affects the CMB power spectrum, but this is limited to large-scale perturbations through the ISW effect (which is bounded by the cosmic variance). In other words, the matter power spectrum corresponding to the scales (12.96) is subject to the modification of gravity, while the CMB power spectrum on these scales is hardly affected. From Eq. (12.115), we have $\Delta n_s = 0.074$ for $n = 1$ and $\Delta n_s = 0.047$ for $n = 2$. In current observations, we have not seen any discrepancies between the two power spectra. If we take the conservative bound $\Delta n_s < 0.5$, it follows that $n \geq 2$ [21]. The Λ CDM model can be regarded as the limit $n \rightarrow \infty$, in which case $\Delta n_s \rightarrow 0$.

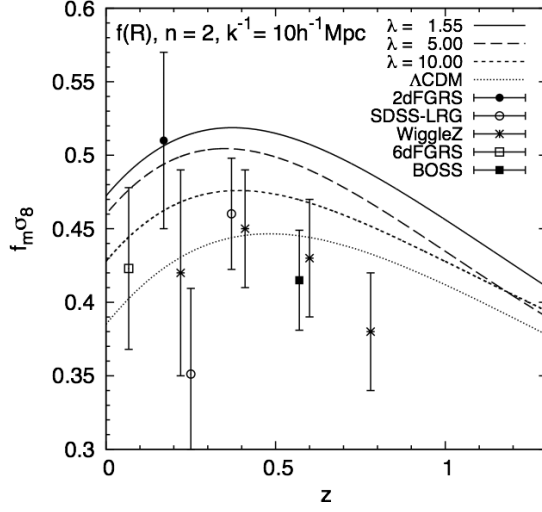


Fig. 12.1. Evolution of $f_m \sigma_8$ versus the redshift z for the $f(R)$ model (11.14) with the scale $k^{-1} = 10 h^{-1} \text{Mpc}$. The model parameters are chosen to be $n = 2$, $\sigma_8(z = 0) = 0.811$, and $\Omega_{\text{DE}}^{(0)} = 0.72$. The solid, long dashed, dashed curves are the theoretical predictions for the cases $\lambda = 1.55, 5, 10$, respectively, whereas the dotted curve corresponds to the Λ CDM model. We also plot the observational data of $f_m \sigma_8$ constrained from RSD measurements. Reproduced from Ref. [33].

From Eq. (12.113), z_k also depends on the model parameter λ . For larger λ the transition to the regime $M_\phi^2 < k^2/a^2$ occurs at later cosmological epochs, so the modification of gravity tends to be less significant. In Fig. 12.1, we plot the evolution of $f_m \sigma_8$ for the scale $k = 0.1 h \text{Mpc}^{-1}$ and $n = 2$ with several different values of λ , where $f_m \equiv \dot{\delta}_m / (H \delta_m)$ is the growth rate of matter perturbations. For larger λ the values of $f_m \sigma_8$ tend to be smaller for $z < 1$, which reflects the fact that the transition redshift z_k gets smaller. The current RSD data shown in Fig. 12.1 is not sufficiently accurate to distinguish between the models with different values of λ . Still, for $n = 2$, the models with λ of the order of unity are in tension with the RSD data [33].

The above discussion is valid in the linear regime characterized by Eq. (12.96), but non-linear effects such as the mode-mode coupling between different wave numbers become important for $k \gtrsim 0.2 h \text{Mpc}^{-1}$. In Refs. [34–38], the numerical codes of N -body simulations were developed for the $f(R)$ model (11.14). On smaller scales, the screening mechanism of fifth forces — dubbed the chameleon mechanism [39, 40] — is implemented in the code to recover the gravitational interaction close to that of GR (as we will discuss in Chap. 14). While the matter power spectrum in the quasi-nonlinear regime is enhanced relative to the GR case, the chameleon mechanism tends to suppress the enhancement of the matter power spectrum in the fully non-linear regime ($k \gtrsim 1 h \text{Mpc}^{-1}$).

12.4.2. Brans–Dicke theories

The next example is BD theory given by the action (11.45). In Sec. 11.2.1, we already showed that, under the no-ghost condition $\omega_{\text{BD}} > -3/2$, the action is equivalent to Eq. (11.63) with the correspondences $\chi = e^{-2Q\phi/M_{\text{pl}}}$ and $3 + 2\omega_{\text{BD}} = 1/(2Q^2)$. In the following, we employ the action (11.63) for discussing theoretically consistent conditions and the evolution of cosmological perturbations in BD theory. In terms of the language of Horndeski theories, the action (11.63) corresponds to the following functions

$$G_2 = (1 - 6Q^2) e^{-2Q\phi/M_{\text{pl}}} X - V(\phi), \quad G_4 = \frac{M_{\text{pl}}^2}{2} e^{-2Q\phi/M_{\text{pl}}}, \quad G_3 = 0 = G_5. \quad (12.116)$$

We recall that the quantity Q characterizes the coupling between the scalar field and non-relativistic matter in the Einstein frame. The minimally coupled quintessence can be recovered in the limit that $Q \rightarrow 0$. For the functions (12.116), the quantities (12.32)–(12.35) read

$$\begin{aligned} w_1 = w_4 &= M_{\text{pl}}^2 e^{-2Q\phi/M_{\text{pl}}}, & w_2 &= 2M_{\text{pl}} e^{-2Q\phi/M_{\text{pl}}} (M_{\text{pl}} H - Q\dot{\phi}), \\ w_3 &= \frac{3}{2} e^{-2Q\phi/M_{\text{pl}}} \left[(1 - 6Q^2) \dot{\phi}^2 + 6M_{\text{pl}} (2QH\dot{\phi} - M_{\text{pl}} H^2) \right]. \end{aligned} \quad (12.117)$$

The background equations are given by Eqs. (11.89) and (11.90) with $F = e^{-2Q\phi/M_{\text{pl}}}$, which also follow from Eqs. (12.19) and (12.20) after substitutions of the functions (12.116). Then, the quantities associated with conditions for the absence of ghosts and Laplacian instabilities read

$$Q_t = \frac{1}{4} M_{\text{pl}}^2 F, \quad c_t^2 = 1, \quad (12.118)$$

and

$$Q_s = \frac{F M_{\text{pl}}^2 \dot{\phi}^2}{2(M_{\text{pl}} H - Q\dot{\phi})^2}, \quad c_s^2 = 1. \quad (12.119)$$

Since the quantity $F = e^{-2Q\phi/M_{\text{pl}}}$ is positive under the condition (11.57), there are neither ghosts nor Laplacian instabilities for $\omega_{\text{BD}} > -3/2$.

From Eqs. (12.73), (12.74) and (12.79), the effective gravitational coupling, the gravitational slip parameter, and the quantity $\mathcal{F}$ reduce, respectively, to [23]

$$G_{\text{eff}} = \frac{G}{F} \frac{(1 + 2Q^2)F + (M_{\phi} a/k)^2}{F + (M_{\phi} a/k)^2}, \quad (12.120)$$

$$\eta = \frac{(1 - 2Q^2)F + (M_{\phi} a/k)^2}{(1 + 2Q^2)F + (M_{\phi} a/k)^2}, \quad (12.121)$$

$$\mathcal{F} = \frac{1}{F}. \quad (12.122)$$

In the regime where the scalar field is sufficiently massive such that the condition $M_\phi^2/F \gg k^2/a^2$ is satisfied, we have $G_{\text{eff}} \simeq G/F$ and $\eta \simeq 1$. For F close to 1, the evolution of perturbations in this regime is similar to that of GR. For $M_\phi^2/F \ll k^2/a^2$, it follows that

$$G_{\text{eff}} \simeq \frac{G}{F}(1 + 2Q^2) = \frac{G}{F} \frac{4 + 2\omega_{\text{BD}}}{3 + 2\omega_{\text{BD}}}, \quad (12.123)$$

$$\eta \simeq \frac{1 - 2Q^2}{1 + 2Q^2} = \frac{1 + \omega_{\text{BD}}}{2 + \omega_{\text{BD}}}, \quad (12.124)$$

where we used the correspondence (11.62). This can be regarded as the “scalar–tensor regime” in which the effect of modification of gravity manifests itself for the growth of matter perturbations. The metric $f(R)$ gravity corresponds to $Q = -1/\sqrt{6}$ (or $\omega_{\text{BD}} = 0$), so that $G_{\text{eff}} \simeq 4G/(3F)$ and $\eta \simeq 1/2$. The effective gravitational potential ψ_{eff} in Eq. (12.78) is affected by the modified evolution of the matter density contrast δ_m .

If we transform the action (11.63) to that in the Einstein frame, the resulting theory corresponds to the coupled quintessence scenario described by the action (10.113) with the coupling Q . In Sec. 10.3.1, we studied the cosmological dynamics of coupled quintessence for the exponential potential $\hat{V}(\phi) = V_0 e^{-\lambda\phi/M_{\text{Pl}}}$. On using Eqs. (11.60) and (11.61), the corresponding potential in the Jordan frame is given by $V(\phi) = V_0 e^{-\mu\phi/M_{\text{Pl}}}$, where $\mu = \lambda + 4Q$. In this case the second derivative $V_{,\phi\phi}$, which is of the order of M_ϕ^2 , can be estimated as $V_{,\phi\phi} = \mu^2 V/M_{\text{Pl}}^2 \approx \mu^2 H^2 \Omega_\phi$, where $\Omega_\phi \approx V/(M_{\text{Pl}}^2 H^2)$ is the field density parameter. Since μ is at most of the order of unity for realizing the late-time cosmic acceleration, the mass squared M_ϕ^2 does not exceed the order of H^2 . For sub-horizon modes ($k^2/a^2 \gg H^2$), the perturbations are always in the scalar–tensor regime ($M_\phi^2/F \ll k^2/a^2$) for the exponential potential.

If the field mass is always light as in the case of the exponential potential, the scalar field mediates the fifth force with matter. If the coupling $|Q|$ is larger than the order of 10^{-3} , this contradicts with the local gravity experiments in the solar system. In Sec. 10.3.1, the setup is the Einstein-frame action in which it is assumed that the scalar field interacts only with dark matter. Now, our starting point is the Jordan-frame action (11.63), so it is inevitable to avoid the interaction between the scalar field and baryons. As we will discuss in Chap. 13, if the scalar field has a large mass in regions of high density, it is possible to suppress the propagation of fifth forces through the chameleon mechanism [39, 40]. The example of such a potential is given by Eq. (11.88), i.e.,

$$V(\phi) = V_0 \left[1 - C(1 - e^{-2Q\phi/M_{\text{Pl}}})^p \right], \quad (12.125)$$

where $0 < p < 1$.

For the potential (12.125), the field evolves slowly along the instantaneous minimum ϕ_m given by Eq. (11.94). Since ϕ_m is close to 0 in the early cosmological epoch, the field dynamics mimics that of the Λ CDM model with $V(\phi) \simeq V_0$.

After ρ_m drops down to the order of V_0 , ϕ_m starts to be away from 0. Unlike the coupled quintessence with the exponential potential, there exists no ϕ MDE with constant Ω_ϕ . During the matter era, the mass squared M_ϕ^2 around $\phi = \phi_m$ is approximately given by

$$M_\phi^2 \simeq V_{,\phi\phi} \simeq \frac{1-p}{(2^p p C)^{1/(1-p)}} Q^2 \left(\frac{\rho_m}{V_0} \right)^{(2-p)/(1-p)} V_0, \quad (12.126)$$

which decreases as $M_\phi^2 \propto t^{-2(2-p)/(1-p)}$. As we go back to the past, M_ϕ^2 dominates over the term k^2/a^2 (which is proportional to $t^{-4/3}$), so there is the time t_k at which M_ϕ^2/F is equivalent to k^2/a^2 . If this transition occurs in the matter era, the critical redshift z_k can be estimated as

$$z_k \simeq \left[\left(\frac{k}{a_0 H_0} \frac{1}{|Q|} \right)^{2(1-p)} \frac{2^p p C}{(1-p)^{1-p}} \frac{1}{(3F_0 \Omega_m^{(0)})^{2-p}} \frac{V_0}{H_0^2} \right]^{\frac{1}{4-p}} - 1, \quad (12.127)$$

where the subscript “0” represents today’s values. From Eq. (12.127), the time t_k has the dependence $t_k \propto k^{-\frac{3(1-p)}{4-p}}$. For larger k and smaller p , the transition to the regime $M_\phi^2/F < k^2/a^2$ occurs earlier.

Under the quasi-static approximation on sub-horizon scales, the matter perturbation obeys Eq. (12.51). This approximation is trustable as long as the oscillating mode of the field perturbation $\delta\phi$ is initially suppressed relative to the matter-induced mode. For $t < t_k$, the density contrast evolves as $\delta_m \propto t^{2/3}$. For $t > t_k$, the matter perturbation Eq. (12.51) reduces to

$$\frac{d^2 \delta_m}{d\mathcal{N}^2} + \left(\frac{1}{2} - \frac{3}{2} w_{\text{eff}} \right) \frac{d\delta_m}{d\mathcal{N}} - \frac{3}{2} \Omega_m (1 + 2Q^2) \delta_m \simeq 0, \quad (12.128)$$

where $\mathcal{N} = \ln a$ and $\Omega_m = \rho/(3M_{\text{pl}}^2 H^2 F)$. This equation has the following growing-mode solution during the matter dominance ($w_{\text{eff}} \simeq 0$ and $\Omega_m \simeq 1$):

$$\delta_m \propto t^{(\sqrt{25+48Q^2}-1)/6}. \quad (12.129)$$

For increasing $|Q|$, the growth rate $f_m \equiv \dot{\delta}_m/(H\delta_m) = (\sqrt{25+48Q^2}-1)/4$ gets larger. The modification of gravity strongly manifests itself in RSD measurements ($z \lesssim 1.5$) for z_k greater than the order of 1. As it happens in $f(R)$ gravity ($Q = -1/\sqrt{6}$), the larger growth of δ_m with $|Q| = \mathcal{O}(1)$ tends to be more difficult to be compatible with the RSD data. The current observational constraint on the growth rate is weak, but we may take the criterion $f_m \lesssim 2$ from several measurements. In this case, the analytic solution (12.129) gives the upper bound $Q < 1.08$ [41, 42].

On using the solution (12.129), the matter power spectrum P_{δ_m} at the onset of cosmic acceleration ($t = t_{\text{DE}}$) is different from that in the Λ CDM model, as

$$\frac{P_{\delta_m}(t_{\text{DE}})}{P_{\delta_m}^{\Lambda\text{CDM}}(t_{\text{DE}})} = \left(\frac{t_{\text{DE}}}{t_k}\right)^{2\left(\frac{\sqrt{25+48Q^2}-1}{6}-\frac{2}{3}\right)} \propto k^{\Delta n_s}, \quad (12.130)$$

where

$$\Delta n_s = \frac{(1-p)(\sqrt{25+48Q^2}-5)}{4-p}. \quad (12.131)$$

Analogous to the discussion in Sec. 12.4.1, this leads to the difference Δn_s between the spectral indices of the matter power spectrum and the CMB spectrum on the scales (12.96). As long as p is close to 1, Δn_s is close to 0, so the model can be consistent with the observations of the two power spectra. In $f(R)$ models (11.14) and (11.15), this amounts to choosing n larger than the order of 1.

The weak lensing is another tool for probing modified gravitational theories. The effective density field δ_{eff} is related to the effective weak lensing gravitational potential ψ_{eff} according to Eq. (8.95). In Brans–Dicke theories, ψ_{eff} obeys Eq. (12.78) with $\mathcal{F} = 1/F$ under the quasi-static approximation on sub-horizon scales. Defining the matter density parameter as $\Omega_m^{(0)} = 8\pi G\rho_0/(3H_0^2 F_0)$, where F_0 is the today's value of F , we obtain the relation [24, 43, 44]

$$\delta_{\text{eff}} = \frac{F_0}{F} \delta_m. \quad (12.132)$$

In Sec. 8.7, we derived the convergence power spectrum in the form (8.105). Now, the power spectrum $P_{\delta_{\text{eff}}}$ of the density field is related to the matter power spectrum P_{δ_m} as $P_{\delta_{\text{eff}}} = (F_0/F)^2 P_{\delta_m}$, so the convergence spectrum yields

$$P_\kappa(l) = \left(\frac{3H_0^2\Omega_m^{(0)}}{2}\right)^2 \int_0^\infty dr \left(\frac{g(r)}{a(r)}\right)^2 \left(\frac{F_0}{F}\right)^2 P_{\delta_m}(l/r, r), \quad (12.133)$$

where the function $g(r)$ is defined by Eq. (8.98) with the coming distance $r(z) = \int_0^z d\tilde{z}/H(\tilde{z})$. Assuming that the source is located at $r = r_s$, we can take the distribution function $n(r') = \delta(r' - r_s)$ and hence $g(r) = (r_s - r)/r_s$. In this case, Eq. (12.133) reduces to

$$P_\kappa(l) = \left(\frac{3H_0^2\Omega_m^{(0)}}{2}\right)^2 \int_0^{r_s} dr \left(\frac{r_s - r}{r_s a} \frac{F_0}{F}\right)^2 P_{\delta_m}(l/r, r). \quad (12.134)$$

The matter power spectrum P_{δ_m} is affected by the modification of gravity, so that the convergence power spectrum is also subject to change.

In Fig. 12.2, we plot the convergence power spectrum in BD theories with the potential (12.125) for two different values of Q . For increasing $|Q|$, the power spectrum tends to be enhanced relative to that of the Λ CDM model. The enhancement is especially significant for larger multipoles $\ell = k/r$. This reflects the fact that the

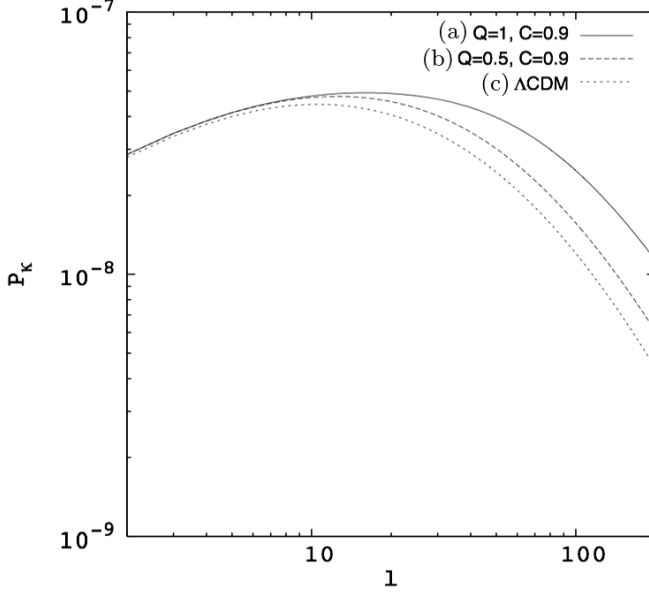


Fig. 12.2. The convergence power spectrum $P_\kappa(\ell)$ for (a) $Q=1, p=0.7, C=0.9$, (b) $Q=0.5, p=0.7, C=0.9$, and (c) the Λ CDM model. The other model parameters are chosen to be $\Omega_m^{(0)} = 0.28$ and $H_0 = 3.34 \times 10^{-4} h \text{ Mpc}^{-1}$ with the primordial curvature perturbation $\mathcal{P}_\mathcal{R} = 2.0 \times 10^{-9}$ and the scalar spectral index $n_s = 1$. Reproduced from Ref. [43].

transition to the regime $M_\phi^2/F < k^2/a^2$ occurs earlier for smaller-scale perturbations. The cosmic shear data from the CFHTLenS survey showed that the $f(R)$ model (11.17) with $n = 1/2$ and $f_{,R}(z=0) = 10^{-4}$ is excluded at more than 99.9% CL [45]. The current weak lensing measurements are not yet sufficiently accurate to distinguish models with different values of Q , but it is expected that this situation will be improved in the future.

12.4.3. Covariant Galileons

The action (11.165) of covariant Galileons corresponds to the choices of functions

$$G_2 = -c_2 X, \quad G_3 = \frac{c_3}{M^3} X, \quad G_4 = \frac{1}{2} M_{\text{pl}}^2 - \frac{c_4}{M^6} X^2, \quad G_5 = \frac{3c_5}{M^9} X^2, \quad (12.135)$$

where c_i 's ($i = 2, 3, 4, 5$) are dimensionless constants and M is a constant having the dimension of mass. Note that we do not take into account the linear potential ϕ in G_2 .

In Sec. 11.3.4, we showed the existence of late-time de Sitter solutions satisfying the conditions (11.175) and (11.176), where $x_{\text{dS}} = \dot{\phi}_{\text{dS}}/(H_{\text{dS}} M_{\text{pl}})$, $\alpha = c_4 x_{\text{dS}}^4$, and $\beta = c_5 x_{\text{dS}}^5$. As we will see below, the quantities $|\alpha|$ and $|\beta|$ are at most of the order of unity for theoretically consistent parameter spaces. The mass M is normalized to be

$M^3 = M_{\text{pl}} H_{\text{dS}}^2$. We recall that the variables $r_1 = \dot{\phi}_{\text{dS}} H_{\text{dS}} / (\dot{\phi} H)$, $r_2 = (\dot{\phi} / \dot{\phi}_{\text{dS}})^4 / r_1$, and $\Omega_r = \rho_r / (3M_{\text{pl}}^2 H^2)$ obey the differential equations (11.180)–(11.182), respectively. For the derivation of theoretically consistent conditions, we take into account both non-relativistic matter and radiation.

For tensor perturbations, the quantities Q_t and c_t^2 defined by Eq. (12.57) can be expressed, respectively, as [46, 47]

$$Q_t = \frac{1}{8} M_{\text{pl}}^2 (2 + 3\alpha r_1 r_2 - 6\beta r_2), \quad (12.136)$$

$$c_t^2 = \frac{2r_1(2 - \alpha r_1 r_2) - 3\beta(r_2 r_1' + r_1 r_2')}{2r_1(2 + 3\alpha r_1 r_2 - 6\beta r_2)}, \quad (12.137)$$

where a prime represents a derivative with respect to $\mathcal{N} = \ln a$. For scalar perturbations, the quantities Q_s and c_s^2 given by Eqs. (12.68) and (12.71) reduce, respectively, to

$$Q_s = -\frac{s M_{\text{pl}}^2}{(1 + \mu_3)^2}, \quad (12.138)$$

$$c_s^2 = \{ (1 + \mu_1)^2 [2\mu_3' - (1 + \mu_3)(5 + 3w_{\text{eff}}) + 4\Omega_r + 3\Omega_m] - 4\mu_1'(1 + \mu_1)(1 + \mu_2) + 2(1 + \mu_3)^2(1 + \mu_4) \} / (2s), \quad (12.139)$$

where

$$s \equiv 3(1 + \mu_1)(\mu_1 + \mu_2 + \mu_1\mu_2 - 2\mu_3 - \mu_3^2), \quad (12.140)$$

$$\mu_1 \equiv 3\alpha r_1 r_2 / 2 - 3\beta r_2, \quad (12.141)$$

$$\mu_2 \equiv (3\alpha - 4\beta + 2)r_1^3 r_2 / 2 - 2(9\alpha - 9\beta + 2)r_1^2 r_2 + 45\alpha r_1 r_2 / 2 - 28\beta r_2, \quad (12.142)$$

$$\mu_3 \equiv -(9\alpha - 9\beta + 2)r_1^2 r_2 / 2 + 15\alpha r_1 r_2 / 2 - 21\beta r_2 / 2, \quad (12.143)$$

$$\mu_4 \equiv -\alpha r_1 r_2 / 2 - 3\beta r_2 (r_1' / r_1 + r_2' / r_2) / 4. \quad (12.144)$$

In Sec. 11.3.4, we showed the existence of tracker solutions characterized by $r_1 = 1$. The tracker is in tension with the observational data of SN Ia, CMB, and BAO due to the large deviation of w_{DE} from -1 during the matter era. However, the solutions approaching the tracker at low redshifts are allowed from the data. In this case, the solutions satisfy the conditions $r_1 \ll 1$ and $r_2 \ll 1$ in the early cosmological epoch before reaching the tracker. In the regime where both r_1 and r_2 are much smaller than 1, the quantities associated with tensor perturbations reduce, respectively, to

$$Q_t \simeq \frac{1}{4} M_{\text{pl}}^2, \quad (12.145)$$

$$c_t^2 \simeq 1 + \frac{3}{8} \beta r_2 (5 - 3\Omega_r) \simeq 1, \quad (12.146)$$

which are both positive. From Eqs. (12.138) and (12.139), we obtain

$$Q_s \simeq 30M_{\text{pl}}^2\beta r_2, \quad (12.147)$$

$$c_s^2 \simeq \frac{1}{40}(1 + \Omega_r). \quad (12.148)$$

For $r_2 > 0$, we require that $\beta > 0$ to avoid the scalar ghost. Since c_s^2 is positive, there is no Laplacian instability of scalar perturbations.

Let us derive theoretically consistent conditions after the solutions enter the tracking regime ($r_1 = 1$). In the regime $r_2 \ll 1$, we have

$$Q_t \simeq \left[\frac{1}{4} + \frac{3}{8}(\alpha - 2\beta)r_2 \right] M_{\text{pl}}^2 \simeq \frac{1}{4}M_{\text{pl}}^2, \quad (12.149)$$

$$c_t^2 \simeq 1 - \frac{1}{2}(4\alpha + 3\beta + 3\beta\Omega_r)r_2 \simeq 1, \quad (12.150)$$

which are both positive, and

$$Q_s \simeq \frac{3}{2}(2 - 3\alpha + 6\beta)M_{\text{pl}}^2r_2, \quad (12.151)$$

$$c_s^2 \simeq \frac{8 + 10\alpha - 9\beta + \Omega_r(2 + 3\alpha - 3\beta)}{3(2 - 3\alpha + 6\beta)}. \quad (12.152)$$

For the branch $r_2 > 0$, the condition $Q_s > 0$ translates to

$$2 - 3\alpha + 6\beta > 0. \quad (12.153)$$

With this condition, c_s^2 is positive for

$$8 + 10\alpha - 9\beta + \Omega_r(2 + 3\alpha - 3\beta) > 0. \quad (12.154)$$

At the de Sitter solution ($r_1 = 1, r_2 = 1$), the theoretically consistent conditions are given by

$$Q_t = \frac{1}{8}M_{\text{pl}}^2(2 + 3\alpha - 6\beta) > 0, \quad (12.155)$$

$$c_t^2 = \frac{2 - \alpha}{2 + 3\alpha - 6\beta} > 0, \quad (12.156)$$

and

$$Q_s = \frac{4 - 9(\alpha - 2\beta)^2}{6(\alpha - 2\beta)^2}M_{\text{pl}}^2 > 0, \quad (12.157)$$

$$c_s^2 = \frac{(\alpha - 2\beta)(4 + 15\alpha^2 - 48\alpha\beta + 36\beta^2)}{2[4 - 9(\alpha - 2\beta)^2]} > 0. \quad (12.158)$$

We also consider the intermediate regime between $r_2 \ll 1$ and $r_2 = 1$. Provided that the conditions $Q_t > 0$, $Q_s > 0$, and $c_s^2 > 0$ are satisfied both in the regimes $r_2 \ll 1$ and $r_2 = 1$, these conditions are not violated in the intermediate epoch.

On the other hand, c_t^2 can be negative during the transition from $r_2 \ll 1$ to $r_2 = 1$ [46, 47]. Since the quantity r_2 obeys the differential equation (11.187) along the tracker, the tensor propagation speed squared (12.137) reads

$$c_t^2 = \frac{2 + (2 - \alpha - 9\beta)r_2 + (9\beta - \alpha)r_2^2}{(1 + r_2)[2 + 3(\alpha - 2\beta)r_2]}, \quad (12.159)$$

where we have dropped the contribution from the term Ω_r (because the transition to the de Sitter solution occurs only recently). Then, c_t^2 has an extremum at

$$r_{2m} = \frac{4\alpha - 15\beta \pm 3\sqrt{\beta(30\beta - 8\alpha + 12\alpha^2 - 15\alpha\beta - 18\beta^2)}}{15\beta - 4\alpha + 27\alpha\beta - 54\beta^2}. \quad (12.160)$$

For positive values of α and β larger than 1, the tensor propagation speed squared (12.159) tends to be negative for the plus sign of r_{2m} . When $\alpha = 2$ and $\beta = 1.2$, for example, we have $c_t^2 = -0.65$ and $r_{2m} = 0.64$. For smaller α and β , c_t^2 can be positive, e.g., $c_t^2 = 0.36$ and $r_{2m} = 0.60$ for $\alpha = 1$ and $\beta = 0.5$. For $\beta > 0$ and the plus sign of Eq. (12.160), the condition $c_t^2(r_{2m}) > 0$ translates to

$$2\beta < \alpha < 12\sqrt{\beta} - 9\beta - 2. \quad (12.161)$$

In Fig. 12.3, we plot the parameter space constrained by the conditions (12.153)–(12.158) and (12.161). The four borders in the viable parameter space correspond to (i) the condition (12.153), (ii) the condition (12.154) at $\Omega_r = 1$, (iii) the condition $\alpha > 2\beta$ following from (12.158), and (iv) the condition (12.161).

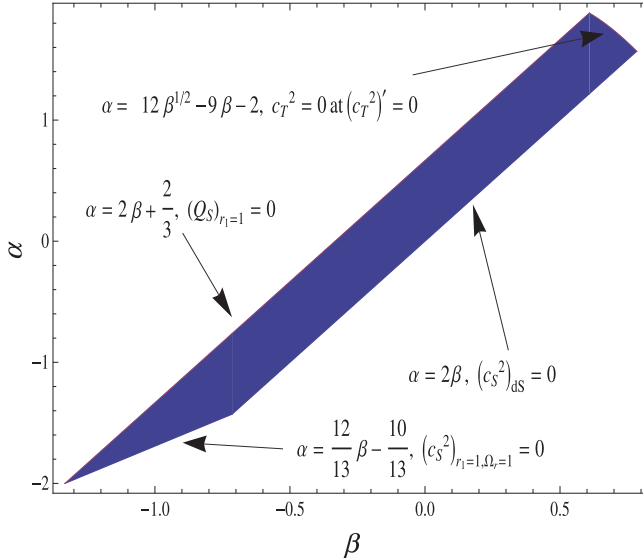


Fig. 12.3. Theoretically viable parameter space (shown as a black color) in the (α, β) plane for covariant Galileons with the branch $r_2 > 0$. The coefficients c_2 and c_3 are related to α and β according to (11.175) and (11.176). Reproduced from Ref. [46].

If the initial conditions are close to those of the tracker ($r_1 \simeq 1, r_2 \ll 1$), then the parameters α and β need to be inside the black region shown in Fig. 12.3. For late-time tracking solutions, the initial conditions correspond to $r_1 \ll 1$ and $r_2 \ll 1$, in which case the condition

$$\beta > 0, \quad (12.162)$$

is also required for the branch $r_2 > 0$ to avoid the scalar ghost.

In the following, we study the evolution of non-relativistic matter perturbations to see observational signatures of covariant Galileons. Since we are considering field derivative couplings without the potential, we can set M_ϕ^2 to 0 for deriving the effective gravitational coupling G_{eff} and the gravitational slip parameter η . Under the quasi-static approximation on sub-horizon scales, G_{eff} and η are given, respectively, by Eqs. (12.82) and (12.83), both of which are independent of k .

In the three different regions (i) $r_1 \ll 1, r_2 \ll 1$, (ii) $r_1 = 1, r_2 \ll 1$, and (iii) $r_1 = 1, r_2 = 1$, we can analytically estimate G_{eff} and η as follows [28].

(i) $r_1 \ll 1, r_2 \ll 1$

Expanding Eqs. (12.82) and (12.83) around $r_1 = 0, r_2 = 0$, it follows that

$$\frac{G_{\text{eff}}}{G} \simeq 1 + \frac{255}{8}\beta r_2, \quad (12.163)$$

$$\eta \simeq 1 + \frac{129}{8}\beta r_2. \quad (12.164)$$

For the branch $r_2 > 0$ we require that $\beta > 0$ to avoid scalar ghosts, so we have $G_{\text{eff}} > G$ and $\eta > 1$ in this regime.

(ii) $r_1 = 1, r_2 \ll 1$

For $r_1 = 1$, expansion of G_{eff} and η about $r_2 = 0$ leads to

$$\frac{G_{\text{eff}}}{G} \simeq 1 + \frac{291\alpha^2 + 702\beta^2 - 933\alpha\beta + 20\alpha - 84\beta + 4}{2(10\alpha - 9\beta + 8)}r_2, \quad (12.165)$$

$$\eta \simeq 1 - \frac{3(126\alpha^2 + 306\beta^2 - 405\alpha\beta + 4\alpha - 30\beta)}{2(10\alpha - 9\beta + 8)}r_2, \quad (12.166)$$

which depend on both α and β .

(iii) $r_1 = 1, r_2 = 1$

At the de Sitter solution, we have

$$\frac{G_{\text{eff}}}{G} = \frac{1}{3(\alpha - 2\beta)}, \quad \eta = 1. \quad (12.167)$$

The latter means that Φ is equivalent to $-\Psi$.

Since the late-time tracking solutions are favored from observational constraints at the background level [48], the solutions start from the regime (i), temporally enter the regime (ii), and finally approach the de Sitter fixed point (iii). In Fig. 12.4, we show one example for the evolution of δ_m/a and ψ_{eff} with the model parameters

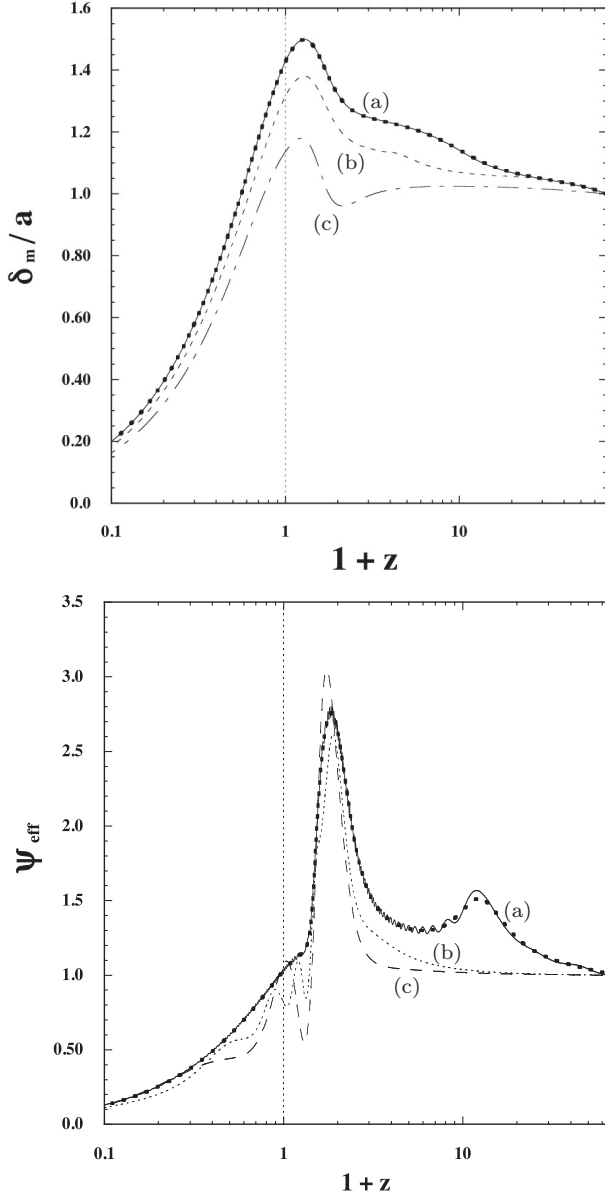


Fig. 12.4. Evolution of cosmological perturbations versus $1+z$ for $\alpha = 1.37$ and $\beta = 0.44$ with the initial conditions $r_1 = 0.03$ and $r_2 = 0.003$ at $z = 70$. (Top) Variations of δ_m/a for the wave numbers (a) $k = 300a_0H_0$, (b) $k = 30a_0H_0$, and (c) $k = 5a_0H_0$. (Bottom) Variations of ψ_{eff} for the wave numbers (a) $k = 300a_0H_0$, (b) $k = 10a_0H_0$, and (c) $k = 5a_0H_0$. Both δ_m/a and ψ_{eff} are divided by their initial amplitudes $\delta_m(t_i)/a(t_i)$ and $\psi_{\text{eff}}(t_i)$, respectively. The bold dotted lines are derived under the quasi-static approximation on sub-horizon scales. Reproduced from Ref. [28].

$\alpha = 1.37$ and $\beta = 0.44$. The initial conditions of r_1 and r_2 are chosen such that the solutions approach the tracker at late times. In this case, the analytic estimations (12.163)–(12.167) show that $G_{\text{eff}}/G \simeq 1 + 14.0r_2$, $\eta \simeq 1 + 7.10r_2$ in the regime (i), $G_{\text{eff}}/G \simeq 1 + 3.22r_2$, $\eta \simeq 1 - 3.71r_2$ in the regime (ii), and $G_{\text{eff}}/G \simeq 0.68$, $\eta = 1$ in the regime (iii). Hence G_{eff} is larger than G for $r_2 \ll 1$, but it starts to decrease as the solutions approach the de Sitter attractor.

For the modes $k/(a_0 H_0) > \mathcal{O}(100)$, the results derived under the quasi-static approximation exhibit good agreement with those obtained by the integration of full perturbation equations of motion. In Fig. 12.4, we observe that the difference arises for the modes $k/(a_0 H_0) < \mathcal{O}(10)$. For smaller k , the growth of δ_m tends to be less significant. For the modes (12.96) relevant to the observations of large-scale structures, the matter perturbation δ_m grows faster than that in GR during the matter era ($\delta_m \propto a$).

In the bottom panel of Fig. 12.4 we find that, for the modes $k/(a_0 H_0) > \mathcal{O}(100)$, the effective gravitational potential ψ_{eff} varies even in the deep matter era. In particular, the quantity $\mathcal{F} = (G_{\text{eff}}/G)(1 + \eta)/2$ appearing in Eq. (12.78) is larger than 1 for $r_2 \ll 1$. This leads to an additional growth of ψ_{eff} to that induced by δ_m . The unusual evolution of ψ_{eff} in covariant Galileons should leave interesting observational signatures in weak lensing observations. At the de Sitter attractor we have $\mathcal{F} = G_{\text{eff}}/G \simeq 0.68$, so ψ_{eff} starts to decrease at some point after the matter dominance.

From the likelihood analysis of using SN Ia, CMB, and BAO data, the parameters α and β are constrained to be $\alpha = 1.404 \pm 0.057$ and $\beta = 0.419 \pm 0.023$ at the background level [48]. In this case, the effective gravitational coupling at the de Sitter attractor is restricted in the range $0.5G < G_{\text{eff}} < 0.72G$. If the model parameters are close to the upper limit $\alpha = 2\beta + 2/3$ of the allowed parameter space shown in Fig. 12.3 (i.e., G_{eff} is close to $0.5G$ at the de Sitter point), the parameter η tends to show a divergence during the transition from the matter era to the epoch of cosmic acceleration [28]. This divergent behavior can be avoided for G_{eff} larger than $0.66G$. For covariant Galileons with de Sitter attractors, the growth rates of δ_m and ψ_{eff} in the past are usually larger than those predicted by the Λ CDM model [28, 33, 49].

In Ref. [50], the authors carried out the full likelihood analysis for covariant Galileons by using the RSD data in addition to the SN Ia, CMB, and BAO data. They did not impose the two relations (11.175) and (11.176) among coefficients $c_{2,3,4,5}$. In such cases there is a tension between constraints from the growth data and those from distance measurements, but there are viable parameter spaces consistent with current observations. It remains to be seen whether upcoming high-precision observational data including weak lensing rule out covariant Galileons or not.

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Chapter 13

Second-order Massive Vector Theories

So far, we have studied the cosmological dynamics and observational consequences in scalar-tensor theories with one scalar degree of freedom (DOF). There are models in which the cosmic acceleration is driven by an Abelian vector field A_μ in the presence of derivative interactions [1–4]. The propagation of such an Abelian vector field is mediated by a spin-1 particle. In general, a massive spin- s particle has $2s + 1$ propagating DOFs. The scalar field is a spin-0 particle, so it has 1 scalar DOF (besides two tensor polarizations in the presence of gravitational interactions).

The photon is a spin-1 particle, so if it is massive, there are three propagating DOFs. Two of them are transverse polarizations associated with electric and magnetic fields, while another is the longitudinal propagation of a scalar DOF. In standard models of particle physics the photon is massless, in which case there exists a $U(1)$ gauge symmetry that forbids the longitudinal propagation. Introduction of the mass term breaks the $U(1)$ gauge invariance such that the longitudinal mode propagates besides two transverse vector polarizations in Minkowski spacetime. The latter massive vector theory is known as a Proca theory.

There have been attempts for constructing theories of Abelian vector fields coupled to gravity [1, 2, 5–7]. If we try to preserve the $U(1)$ gauge invariance for one vector field and stick to second-order equations of motion to avoid Ostrogradski instabilities, there is a no-go theorem stating that the standard Maxwell term $\mathcal{L}_F = -F_{\mu\nu}F^{\mu\nu}/4$, where $F_{\mu\nu} = \nabla_\mu A_\nu - \nabla_\nu A_\mu$, is the only allowed interaction [8]. If we break the $U(1)$ gauge invariance by introducing a mass of the vector field, this allows us to generate derivative interactions similar to those arising for scalar Galileons and Horndeski theories.

In the presence of such vector derivative interactions, it is natural to ask whether they do not modify the number of DOFs in Proca theory. In Ref. [1], Heisenberg constructed the action of generalized Proca theories with second-order equations of motion on curved backgrounds (see also Refs. [2, 9, 10]). The analysis based on the Hessian matrix and the Hamiltonian showed that only three DOFs propagate as in the original Proca theory (besides two tensor polarizations arising from the

gravitational sector). The action of generalized Proca theories contains non-minimal derivative couplings to the Ricci scalar R and the Einstein tensor $G_{\mu\nu}$. Taking the limit $A^\mu \rightarrow \nabla^\mu \pi$, the action of a longitudinal scalar field π reproduces that of a sub-class of Horndeski theories. In generalized Proca theories, two transverse vector modes propagate in addition to the longitudinal mode.

The construction of massive vector theories with derivative interactions is analogous to what was already done for scalar Galileons in Sec. 11.3. In the following, we first build up the action of second-order generalized Proca theories on the Minkowski background and then extend it to that in the curved spacetime.

13.1. Generalized Proca theories in Minkowski spacetime

In the Minkowski spacetime, the Proca theory in the presence of a massive vector field A_μ is given by the action

$$S_{\text{Proca}} = \int d^4x \left(F + m^2 X \right), \quad (13.1)$$

where m is the mass term, and

$$F = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \quad X = -\frac{1}{2} A_\mu A^\mu, \quad (13.2)$$

with the Maxwell tensor $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. Existence of the mass m explicitly breaks the $U(1)$ gauge invariance, such that the longitudinal mode arises besides two transverse polarizations.

Now, we generalize the Proca action (13.1) in such a way that all possible terms containing functions of X as well as derivative self-interactions of A_μ are taken into account. The vector field A_μ has a contribution of the derivative of a scalar field π (called the Stückelberg field) in the form $A_\mu = \partial_\mu \pi + B_\mu$, where B_μ is a divergence-free vector ($\partial_\mu B^\mu = 0$). We would like to build up the action which gives rise to at most second-order equations of motion for both π and A_μ . This demands that the action contains at most second-order derivative terms in π and first-order derivative terms in A_μ . This condition holds for any scalar combination in the action constructed from A_μ , $F_{\mu\nu}$, and the dual strength tensor

$$\tilde{F}^{\mu\nu} = \frac{1}{2} \varepsilon^{\mu\nu\alpha\beta} F_{\alpha\beta}, \quad (13.3)$$

where $\varepsilon^{\mu\nu\alpha\beta}$ is the Levi-Civita tensor defined by Eq. (9.42). Then, the Lagrangian in the form

$$\mathcal{L}_2 = f_2(A_\mu, F_{\mu\nu}, \tilde{F}_{\mu\nu}) \quad (13.4)$$

satisfies the desired property mentioned above.

Derivative interactions similar to those appearing for scalar Galileons can be constructed by using the tensor $\mathcal{B}_{(2n)}^{\mu_1 \dots \mu_n \nu_1 \dots \nu_n}$ given by Eq. (11.124). The scalar

product $\mathcal{B}_{(2n)}^{\mu_1 \dots \mu_n \nu_1 \dots \nu_n} \partial_{\mu_1} A_{\nu_1} \partial_{\mu_2} A_{\nu_2} \dots \partial_{\mu_n} A_{\nu_n}$ in the action gives rise to the equations of motion at most of second order. Even if arbitrary functions $f_{n+2}(X)$ in terms of X are multiplied, the same property is maintained. Then, the Lagrangian densities in the form

$$\mathcal{L}_{n+2} = -\frac{1}{(4-n)!} f_{n+2}(X) \varepsilon^{\mu_1 \dots \mu_n \lambda_1 \dots \lambda_{4-n}} \varepsilon^{\nu_1 \dots \nu_n \lambda_1 \dots \lambda_{4-n}} \partial_{\mu_1} A_{\nu_1} \partial_{\mu_2} A_{\nu_2} \dots \partial_{\mu_n} A_{\nu_n} \quad (13.5)$$

correspond to derivative interactions with at most second-order equations of motion [1, 2]. Analogous to the case of scalar Galileons, there are four terms ($n = 0, 1, 2, 3$) arising from the Lagrangian (13.5). The Lagrangian density $\mathcal{L}_2$ is equivalent to $f_2(X)$. Only for this term, we can consider the more general form (13.4). The Lagrangians (13.5) corresponding to $n = 1, 2, 3$ are given, respectively, by

$$\begin{aligned} \mathcal{L}_3 &= -\frac{1}{3!} f_3(X) \varepsilon^{\mu_1 \lambda_1 \lambda_2 \lambda_3} \varepsilon^{\nu_1 \lambda_1 \lambda_2 \lambda_3} \partial_{\mu_1} A_{\nu_1} \\ &= f_3(X) \partial_\mu A^\mu, \end{aligned} \quad (13.6)$$

$$\begin{aligned} \mathcal{L}_4 &= -\frac{1}{2!} f_4(X) \varepsilon^{\mu_1 \mu_2 \lambda_1 \lambda_2} \varepsilon^{\nu_1 \nu_2 \lambda_1 \lambda_2} \partial_{\mu_1} A_{\nu_1} \partial_{\mu_2} A_{\nu_2} \\ &= f_4(X) [(\partial_\mu A^\mu)^2 - \partial_\rho A_\sigma \partial^\sigma A^\rho], \end{aligned} \quad (13.7)$$

$$\begin{aligned} \mathcal{L}_5 &= -f_5(X) \varepsilon^{\mu_1 \mu_2 \mu_3 \lambda_1} \varepsilon^{\nu_1 \nu_2 \nu_3 \lambda_1} \partial_{\mu_1} A_{\nu_1} \partial_{\mu_2} A_{\nu_2} \partial_{\mu_3} A_{\nu_3} \\ &= f_5(X) [(\partial_\mu A^\mu)^3 - 3\partial_\mu A^\mu \partial_\rho A_\sigma \partial^\sigma A^\rho + 2\partial_\rho A_\sigma \partial^\gamma A^\rho \partial^\sigma A_\gamma]. \end{aligned} \quad (13.8)$$

There are other terms derived by exchanging some of indices in Eqs. (13.7) and (13.8), e.g.,

$$\mathcal{L}_4^V = -\frac{1}{2!} \tilde{f}_4(X) \varepsilon^{\mu_1 \mu_2 \lambda_1 \lambda_2} \varepsilon^{\nu_1 \nu_2 \lambda_1 \lambda_2} \partial_{\mu_1} A_{\mu_2} \partial_{\nu_1} A_{\nu_2}, \quad (13.9)$$

$$\mathcal{L}_5^V = -\tilde{f}_5(X) \varepsilon^{\mu_1 \mu_2 \mu_3 \lambda_1} \varepsilon^{\nu_1 \nu_2 \nu_3 \lambda_1} \partial_{\mu_1} A_{\mu_2} \partial_{\mu_3} A_{\nu_1} \partial_{\nu_2} A_{\nu_3}, \quad (13.10)$$

where $\tilde{f}_4$ and $\tilde{f}_5$ are functions of X . These Lagrangian densities correspond to intrinsic vector modes that vanish by taking the scalar limit $A^\mu \rightarrow \partial^\mu \pi$. The term $\mathcal{L}_4^V$ reduces to

$$\mathcal{L}_4^V = \tilde{f}_4(X) (\partial_\rho A_\sigma \partial^\rho A^\sigma - \partial_\rho A_\sigma \partial^\sigma A^\rho) = -2\tilde{f}_4(X) F, \quad (13.11)$$

which can be absorbed into the Lagrangian density $\mathcal{L}_2$ given by Eq. (13.4). The term $\mathcal{L}_5^V$ contains the intrinsic vector contribution

$$\tilde{\mathcal{L}}_5 = -g_5(X) \tilde{F}^{\alpha\mu} \tilde{F}^\beta{}_\mu \partial_\alpha A_\beta, \quad (13.12)$$

where $g_5(X)$ is a function of X .

For $n = 4$, the Lagrangian density (13.5) gives rise to the sixth-order term

$$\mathcal{L}_6 = -f_6(X)\varepsilon^{\mu_1\mu_2\mu_3\mu_4}\varepsilon^{\nu_1\nu_2\nu_3\nu_4}\partial_{\mu_1}A_{\nu_1}\partial_{\mu_2}A_{\nu_2}\partial_{\mu_3}A_{\nu_3}\partial_{\mu_4}A_{\nu_4}, \quad (13.13)$$

which vanishes in the scalar limit $A^\mu \rightarrow \partial^\mu\pi$. We can also consider another term

$$\mathcal{L}_6^V = -\tilde{f}_6(X)\varepsilon^{\mu_1\mu_2\mu_3\mu_4}\varepsilon^{\nu_1\nu_2\nu_3\nu_4}\partial_{\mu_1}A_{\mu_2}\partial_{\nu_1}A_{\nu_2}\partial_{\mu_3}A_{\nu_3}\partial_{\mu_4}A_{\nu_4}. \quad (13.14)$$

This contains the intrinsic vector contribution

$$\tilde{\mathcal{L}}_6 = -g_6(X)\tilde{F}^{\alpha\beta}\tilde{F}^{\mu\nu}\partial_\alpha A_\mu\partial_\beta A_\nu, \quad (13.15)$$

where $g_6(X)$ is a function of X . In $\mathcal{L}_6^V$ there are also F -dependent terms that can be absorbed into $\mathcal{L}_2$. The series derived from Eq. (13.5) stop at sixth order.

We can also take into account Lagrangian densities containing the products of zeroth and first order derivatives of A_μ , e.g.,

$$\mathcal{L}_4^N = -h_4(X)\varepsilon^{\mu_1\mu_2\mu_3\lambda_1}\varepsilon^{\nu_1\nu_2\nu_3}\lambda_1 A_{\mu_1}A_{\nu_1}\partial_{\mu_2}A_{\nu_2}\partial_{\mu_3}A_{\nu_3}, \quad (13.16)$$

$$\mathcal{L}_5^N = -h_5(X)\varepsilon^{\mu_1\mu_2\mu_3\mu_4}\varepsilon^{\nu_1\nu_2\nu_3\nu_4}A_{\mu_1}A_{\nu_1}\partial_{\mu_2}A_{\nu_2}\partial_{\mu_3}A_{\nu_3}\partial_{\mu_4}A_{\nu_4}. \quad (13.17)$$

After integrations by parts, however, they give rise to interactions same as $\mathcal{L}_4$ and $\mathcal{L}_5$, respectively. Hence we do not need to consider such terms in the Minkowski spacetime. We note that this property does not hold on curved backgrounds. In fact, generalizations of the Lagrangians (13.16) and (13.17) to the curved spacetime generate interactions beyond the framework of second-order generalized Proca theories [11].

In summary, the action of generalized Proca theories whose equations of motion are at most of second order in the Minkowski spacetime is given by [1]

$$S_{\text{GP,Min}} = \int d^4x \left(\sum_{i=2}^5 \mathcal{L}_i + \tilde{\mathcal{L}}_5 + \tilde{\mathcal{L}}_6 \right), \quad (13.18)$$

where $\mathcal{L}_2, \mathcal{L}_{3,4,5}, \tilde{\mathcal{L}}_5, \tilde{\mathcal{L}}_6$ are given, respectively, by Eqs. (13.4), (13.6)–(13.8), (13.12), (13.15). The Lagrangian density $\mathcal{L}_2$ consists of all possible combinations without containing any time derivative of the temporal vector component A_0 . They include the terms like $X, F, XF, F_{\mu\nu}\tilde{F}^{\mu\nu}, A^\mu A^\nu F_\mu{}^\alpha F_{\nu\alpha}$, etc, which do not modify the number of propagating DOFs in the original Proca theory.

To see the absence of the propagation of extra DOFs for Lagrangian densities $\mathcal{L}_i$ higher than quadratic order, we introduce the Hessian matrix $H_{\mu\nu}$ associated with the Lagrangian density $\mathcal{L}$ as

$$H_{\mathcal{L}}^{\mu\nu} = \frac{\partial^2 \mathcal{L}}{\partial \dot{A}_\mu \partial \dot{A}_\nu}. \quad (13.19)$$

To ensure the propagation of three propagating DOFs of A_μ we need to have one constraint equation, which is guaranteed if the determinant of $H_{\mathcal{L}}^{\mu\nu}$ vanishes. In

fact, the cubic Lagrangian density (13.6) obviously gives the vanishing Hessian, so the temporal component A_0 does not propagate.

For the quartic Lagrangian, we consider the sum of three independent interactions in the forms [1, 9]

$$\mathcal{L}_4^{\text{test}} = f_4^{(1)}(X)(\partial_\mu A^\mu)^2 + f_4^{(2)}(X)\partial_\rho A_\sigma \partial^\rho A^\sigma + f_4^{(3)}(X)\partial_\rho A_\sigma \partial^\sigma A^\rho, \quad (13.20)$$

where $f_4^{(i)}(X)$ ($i = 1, 2, 3$) are functions of X . The Hessian matrix derived from this test Lagrangian has only diagonal components:

$$H_{\mathcal{L}_4}^{\mu\nu} = \text{diag}\left(2(f_4^{(1)} + f_4^{(2)} + f_4^{(3)}), -2f_4^{(2)}, -2f_4^{(2)}, -2f_4^{(2)}\right). \quad (13.21)$$

The determinant of $H_{\mathcal{L}_4}^{\mu\nu}$ vanishes for

$$f_4^{(1)} + f_4^{(2)} + f_4^{(3)} = 0. \quad (13.22)$$

We also have another solution $f_4^{(2)} = 0$, but this is not the case we are looking for. Under the condition (13.22) the temporal components of $H_{\mathcal{L}_4}^{\mu\nu}$ vanish, while the three diagonal spatial components are left. On using Eq. (13.22) to eliminate $f_4^{(3)}$, the Lagrangian density (13.20) reads

$$\mathcal{L}_4^{\text{test}} = f_4^{(1)}(X) [(\partial_\mu A^\mu)^2 - \partial_\rho A_\sigma \partial^\sigma A^\rho] + f_4^{(2)}(X) (\partial_\rho A_\sigma \partial^\rho A^\sigma - \partial_\rho A_\sigma \partial^\sigma A^\rho), \quad (13.23)$$

whose first and second contributions are identical to Eqs. (13.7) and (13.11), respectively. Hence the number of propagating DOFs remains three even with the Lagrangians $\mathcal{L}_4$ and $\mathcal{L}_4^V$. Applying the above argument of the Hessian matrix to quintic and sixth-order Lagrangians, it follows that generalized Proca theories with the action (13.18) propagate three propagating DOFs [1, 9].

13.2. Extension to curved spacetime

If we replace partial derivatives in the action (13.18) with covariant derivatives on curved backgrounds, the equations of motion following from $\mathcal{L}_2$ and $\mathcal{L}_3$ are still of second order. However, the Lagrangian densities $\mathcal{L}_4$ and $\mathcal{L}_5$ lead to the equations containing derivatives higher than second order. This situation is analogous to scalar Galileons discussed in Sec. 11.3. We can eliminate higher-order derivative terms by adding non-minimal couplings $G_4(X)R$ and $G_5(X)G_{\mu\nu}\nabla^\mu A^\nu$ in $\mathcal{L}_4$ and $\mathcal{L}_5$, respectively, where $G_4(X)$ and $G_5(X)$ are functions of X . In such cases, the coefficients $f_4(X)$ and $f_5(X)$ in front of Eqs. (13.7) and (13.8) should be chosen as $f_4(X) \rightarrow G_{4,X}(X)$ and $f_5(X) \rightarrow -G_{5,X}(X)/6$, respectively, to avoid the appearance of derivative terms higher than second order. The Lagrangian $\tilde{\mathcal{L}}_5$ does not require any counter term non-minimally coupled to gravity.

Higher-order derivatives arising from $\tilde{\mathcal{L}}_6$ can be removed by adding the term $G_6(X)L^{\mu\nu\alpha\beta}\nabla_\mu A_\nu\nabla_\alpha A_\beta$, where $G_6(X)$ is a function of X and $L^{\mu\nu\alpha\beta}$ is a divergence-free double dual Riemann tensor defined by

$$L^{\mu\nu\alpha\beta} = \frac{1}{4}\epsilon^{\mu\nu\rho\sigma}\epsilon^{\alpha\beta\gamma\delta}R_{\rho\sigma\gamma\delta}. \quad (13.24)$$

Analogous to the Einstein tensor $G_{\mu\nu}$, the divergence-free tensor (13.24) allows one to avoid the appearance of higher-order derivatives of the metric in the equations of motion [9, 10]. In doing so, the coefficient in front of Eq. (13.15) should be chosen as $-g_6(X) \rightarrow G_{6,X}(X)/2$.

In summary, the action of generalized Proca theories whose equations of motion are at most of second order is given by

$$S_{\text{GP}} = \int d^4x \sqrt{-g} \sum_{i=2}^6 \mathcal{L}_i, \quad (13.25)$$

where

$$\mathcal{L}_2 = G_2(A_\mu, F_{\mu\nu}, \tilde{F}_{\mu\nu}), \quad (13.26)$$

$$\mathcal{L}_3 = G_3(X)\nabla_\mu A^\mu, \quad (13.27)$$

$$\mathcal{L}_4 = G_4(X)R + G_{4,X}(X) [(\nabla_\mu A^\mu)^2 - \nabla_\rho A_\sigma \nabla^\sigma A^\rho], \quad (13.28)$$

$$\begin{aligned} \mathcal{L}_5 = & G_5(X)G_{\mu\nu}\nabla^\mu A^\nu - \frac{1}{6}G_{5,X}(X)[(\nabla_\mu A^\mu)^3 - 3\nabla_\mu A^\mu\nabla_\rho A_\sigma\nabla^\sigma A^\rho \\ & + 2\nabla_\rho A_\sigma\nabla^\gamma A^\rho\nabla^\sigma A_\gamma] - g_5(X)\tilde{F}^{\alpha\mu}\tilde{F}^\beta{}_\mu\nabla_\alpha A_\beta, \end{aligned} \quad (13.29)$$

$$\mathcal{L}_6 = G_6(X)L^{\mu\nu\alpha\beta}\nabla_\mu A_\nu\nabla_\alpha A_\beta + \frac{1}{2}G_{6,X}(X)\tilde{F}^{\alpha\mu}\tilde{F}^{\beta\nu}\nabla_\alpha A_\mu\nabla_\beta A_\nu. \quad (13.30)$$

The term $-g_5(X)\tilde{F}^{\alpha\mu}\tilde{F}^\beta{}_\mu\nabla_\alpha A_\beta$ and the Lagrangian density $\mathcal{L}_6$ arise from the intrinsic vector mode. The gauge-invariant vector-tensor interaction derived by Horndeski in 1976 [5] belongs to a sub-class of the action (13.25) with the Lagrangian density $\mathcal{L} = F + \mathcal{L}_4 + \mathcal{L}_6$ with $G_4(X) = M_{\text{pl}}^2/2$ and $G_6(X) = \text{constant}$ (see also Refs. [12, 13] for cosmological applications).

If we take the scalar limit $A^\mu \rightarrow \nabla^\mu\pi$ with $\mathcal{L}_2 = G_2(X)$, the action (13.25) recovers a sub-class of scalar-tensor Horndeski theories [14] in which the functions $G_{2,3,4,5}$ depend on the field derivative $X = -\nabla^\mu\pi\nabla_\mu\pi/2$ alone. In this scalar limit, the term $-g_5(X)\tilde{F}^{\alpha\mu}\tilde{F}^\beta{}_\mu\nabla_\alpha A_\beta$ and $\mathcal{L}_6$ vanish identically. The covariant Galileon corresponds to the specific choices: $G_2 = X, G_3 = X, G_4 = X^2, G_5 = X^2$.

In generalized Proca theories, there are two vector polarizations in addition to the longitudinal scalar mode. Since the gravity sector gives rise to two tensor polarizations, we have five propagating DOFs (one scalar, two vectors, and two tensors) in total.

13.3. Background cosmological dynamics

It is possible to realize the late-time cosmic acceleration in generalized Proca theories. In the following, we study the cosmology given by the action

$$S = S_{\text{GP}} + \int d^4x L_m(g_{\mu\nu}, \Psi_m), \quad (13.31)$$

where Ψ_m are matter fields with the Lagrangian L_m . We assume that the matter sector is minimally coupled to gravity. For the Lagrangian density $\mathcal{L}_2$, we consider the following dependence

$$\mathcal{L}_2 = G_2(X, F, Y), \quad (13.32)$$

where X and F are defined by Eq. (13.2), and

$$Y = A^\mu A^\nu F_\mu{}^\alpha F_{\nu\alpha}. \quad (13.33)$$

It is also possible to include the dependence of the term $F^{\mu\nu} \tilde{F}_{\mu\nu}$ in $\mathcal{L}_2$. Imposing the parity invariance, however, such a term is irrelevant to the dynamics of linear perturbations [15]. Hence we focus on the theories described by Eq. (13.32) with the Lagrangian densities (13.27)–(13.30).

Let us first study the background cosmological dynamics on the flat FLRW background given by the line element $ds^2 = -dt^2 + a^2(t)\delta_{ij}dx^i dx^j$. In order to keep the spatial isotropy of the background, we require that the vector field A^μ has a time-dependent temporal component $\phi(t)$ alone, such that

$$A^\mu = (\phi(t), 0, 0, 0), \quad (13.34)$$

in which case $X = \phi^2/2$. The matter sector obeys the continuity equation (12.21), where ρ and P are the energy density and the isotropic pressure respectively.

Varying the action (13.31) with respect to the metric $g_{\mu\nu}$, we obtain the background equations of motion [4]

$$\begin{aligned} G_2 - G_{2,X}\phi^2 - 3G_{3,X}H\phi^3 + 6G_4H^2 - 6(2G_{4,X} + G_{4,XX}\phi^2)H^2\phi^2 \\ + 5G_{5,X}H^3\phi^3 + G_{5,XX}H^3\phi^5 = \rho, \end{aligned} \quad (13.35)$$

$$\begin{aligned} G_2 - \dot{\phi}\phi^2 G_{3,X} + 2G_4(3H^2 + 2\dot{H}) - 2G_{4,X}\phi(3H^2\phi + 2H\dot{\phi} + 2\dot{H}\phi) \\ - 4G_{4,XX}H\dot{\phi}\phi^3 + G_{5,X}H\phi^2(2\dot{H}\phi + 2H^2\phi + 3H\dot{\phi}) + G_{5,XX}H^2\dot{\phi}\phi^4 = -P. \end{aligned} \quad (13.36)$$

Variation of the action with respect to A^μ leads to

$$\phi(G_{2,X} + 3G_{3,X}H\phi + 6G_{4,X}H^2 + 6G_{4,XX}H^2\phi^2 - 3G_{5,X}H^3\phi - G_{5,XX}H^3\phi^3) = 0, \quad (13.37)$$

which also follows from Eqs. (13.35) and (13.36) by using the matter continuity equation (12.21). We observe that Eq. (13.37) does not contain any time derivative

of ϕ . This reflects the fact that generalized Proca theories are constructed to avoid the propagation of extra DOFs associated with the time derivative of the temporal vector component. The dependence of F, Y in $\mathcal{L}_2$ and the functions $g_5(X), G_6(X)$ does not appear in Eqs. (13.35)–(13.37). This means that the intrinsic vector mode does not affect the background cosmological dynamics.

There are two branches of solutions to Eq. (13.37). The first branch is $\phi = 0$, but in this case the temporal vector component does not contribute to the background dynamics. The second branch is given by

$$G_{2,X} + 3G_{3,X}H\phi + 6G_{4,X}H^2 + 6G_{4,XX}H^2\phi^2 - 3G_{5,X}H^3\phi - G_{5,XX}H^3\phi^3 = 0. \quad (13.38)$$

For this branch there are solutions with non-vanishing ϕ , in which case ϕ is directly related to the Hubble parameter H . Hence it is possible to realize de-Sitter solutions with constant values of H and ϕ . In the following, we will focus on the second branch satisfying Eq. (13.38).

We would like to realize cosmological solutions in which the energy density of ϕ starts to dominate over the background matter density at late times. In doing so, the amplitude of ϕ should grow with the decrease of H . We search for models in which ϕ is related to H according to

$$\phi^p \propto H^{-1}, \quad (13.39)$$

where p is a positive constant. Without losing generality, we focus on the branch of positive ϕ . The solution (13.39) can be realized by considering functions $G_{2,3,4,5}$ containing the power-law dependence of X as

$$\begin{aligned} G_2(X) &= b_2 X^{p_2}, & G_3(X) &= b_3 X^{p_3}, \\ G_4(X) &= \frac{M_{\text{pl}}^2}{2} + b_4 X^{p_4}, & G_5(X) &= b_5 X^{p_5}, \end{aligned} \quad (13.40)$$

where $b_{2,3,4,5}$ are constants, and the powers $p_{3,4,5}$ are given by [4]

$$p_3 = \frac{1}{2}(p + 2p_2 - 1), \quad p_4 = p + p_2, \quad p_5 = \frac{1}{2}(3p + 2p_2 - 1). \quad (13.41)$$

The vector Galileon [1, 2] corresponds to $p_2 = 1$ and $p = 1$, so the temporal vector component has the dependence $\phi \propto H^{-1}$. In what follows, we show that the ansatz (13.39) is indeed consistent with the cosmological dynamics of the model (13.40) with the powers (13.41). For the matter sector, we take into account non-relativistic matter (energy density ρ_m and pressure $P_m = 0$) and radiation (energy density ρ_r and pressure $P_r = \rho_r/3$), so that $\rho = \rho_m + \rho_r$ and $P = \rho_r/3$ in Eqs. (13.35) and (13.36).

To study the background cosmological dynamics, we introduce the density parameters $\Omega_r = \rho_r/(3M_{\text{pl}}^2 H^2)$, $\Omega_m = \rho_m/(3M_{\text{pl}}^2 H^2)$, and $\Omega_{\text{DE}} = 1 - \Omega_r - \Omega_m$.

We also define the dimensionless quantities

$$y \equiv \frac{b_2 \phi^{2p_2}}{3M_{\text{pl}}^2 H^2 2^{p_2}}, \quad \beta_i \equiv \frac{p_i b_i}{2^{p_i - p_2} p_2 b_2} (\phi^p H)^{i-2}, \quad (13.42)$$

where $i = 3, 4, 5$. Under the ansatz (13.39), the terms $\beta_{3,4,5}$ are constant. Then, we can write the field equation (13.38) in the form

$$1 + 3\beta_3 + 6(2p + 2p_2 - 1)\beta_4 - (3p + 2p_2)\beta_5 = 0, \quad (13.43)$$

which may be used to express β_3 in terms of β_4 and β_5 . On account of Eq. (13.35), the dark energy density parameter is related to the quantity y as

$$\Omega_{\text{DE}} = \frac{\beta y}{p_2(p + p_2)}, \quad (13.44)$$

where

$$\beta \equiv -p_2(p + p_2)(1 + 4p_2\beta_5) + 6p_2^2(2p + 2p_2 - 1)\beta_4. \quad (13.45)$$

Differentiating Eq. (13.38) with respect to t and using Eq. (13.36), we can solve them for $\dot{\phi}$ and $\dot{H}$. Then, the density parameters Ω_{DE} and Ω_r obey the differential equations

$$\Omega'_{\text{DE}} = \frac{(1 + s)\Omega_{\text{DE}}(3 + \Omega_r - 3\Omega_{\text{DE}})}{1 + s\Omega_{\text{DE}}}, \quad (13.46)$$

$$\Omega'_r = -\frac{\Omega_r[1 - \Omega_r + (3 + 4s)\Omega_{\text{DE}}]}{1 + s\Omega_{\text{DE}}}, \quad (13.47)$$

where a prime represents the derivative with respect to $\mathcal{N} = \ln a$, and

$$s \equiv \frac{p_2}{p}. \quad (13.48)$$

The terms on the right hand side of Eqs. (13.46) and (13.47) do not diverge for $1 + s > 0$. The effective equation of state $w_{\text{eff}} \equiv -1 - 2\dot{H}/(3H^2)$ can be expressed as

$$w_{\text{eff}} = \frac{\Omega_r - 3(1 + s)\Omega_{\text{DE}}}{3(1 + s\Omega_{\text{DE}})}. \quad (13.49)$$

Writing Eqs. (13.35) and (13.36) in the forms $3M_{\text{pl}}^2 H^2 = \rho + \rho_{\text{DE}}$ and $3M_{\text{pl}}^2 H^2 + 2M_{\text{pl}}^2 \dot{H} = -P - P_{\text{DE}}$ respectively, the dark energy equation of state $w_{\text{DE}} \equiv P_{\text{DE}}/\rho_{\text{DE}}$ yields

$$w_{\text{DE}} = -\frac{3(1 + s) + s\Omega_r}{3(1 + s\Omega_{\text{DE}})}. \quad (13.50)$$

On using Eqs. (13.46) and (13.47), it follows that

$$\frac{\Omega'_{\text{DE}}}{\Omega_{\text{DE}}} = (1 + s) \left(\frac{\Omega'_r}{\Omega_r} + 4 \right). \quad (13.51)$$

This is integrated to give

$$\frac{\Omega_{\text{DE}}}{\Omega_r^{1+s}} = C a^{4(1+s)}, \quad (13.52)$$

where C is a constant. The relation (13.52) is consistent with the solution (13.39). The constant C is known as $C = (\Omega_{\text{DE}}/\Omega_r^{1+s})_0 a_0^{-4(1+s)}$, where the lower subscript “0” represents today’s values. The ratio between Ω_m and Ω_r is given by $\Omega_m/\Omega_r = (a/a_0)(\Omega_m/\Omega_r)_0$, so we can write Eq. (13.52) in the form

$$\frac{\Omega_{\text{DE}} \Omega_r^{3(1+s)}}{(1 - \Omega_{\text{DE}} - \Omega_r)^{4(1+s)}} = \left(\frac{\Omega_{\text{DE}}}{\Omega_r^{1+s}} \right)_0 \left(\frac{\Omega_r}{1 - \Omega_{\text{DE}} - \Omega_r} \right)_0^{4(1+s)}. \quad (13.53)$$

This relation determines the trajectory of solutions in the $(\Omega_{\text{DE}}, \Omega_r)$ plane, which is fixed for given values of $\Omega_{\text{DE}0}$ and Ω_{r0} .

For the dynamical system characterized by the autonomous equations (13.46) and (13.47), we have the following three fixed points:

$$(a) \quad (\Omega_{\text{DE}}, \Omega_r) = (0, 1), \quad w_{\text{eff}} = \frac{1}{3}, \quad w_{\text{DE}} = -1 - \frac{4}{3}s, \quad (13.54)$$

$$(b) \quad (\Omega_{\text{DE}}, \Omega_r) = (0, 0), \quad w_{\text{eff}} = 0, \quad w_{\text{DE}} = -1 - s, \quad (13.55)$$

$$(c) \quad (\Omega_{\text{DE}}, \Omega_r) = (1, 0), \quad w_{\text{eff}} = -1, \quad w_{\text{DE}} = -1, \quad (13.56)$$

which correspond to radiation, matter, and de Sitter fixed points, respectively.

On using Eq. (13.52) in the radiation-dominated epoch, the dark energy density parameter evolves as $\Omega_{\text{DE}} \propto a^{4(1+s)} \propto t^{2(p+p_2)/p}$. Since $\Omega_{\text{DE}} \propto y \propto \phi^{2p_2}/H^2$, the evolution of ϕ is given by $\phi \propto a^{2s/p_2} \propto t^{1/p}$. Since the radiation density parameter during the matter dominance decreases as $\Omega_r \propto a^{-1}$, it follows that $\Omega_{\text{DE}} \propto a^{3(1+s)} \propto t^{2(p+p_2)/p}$. The time dependence of ϕ during the matter era is also the same as that in the radiation era ($\phi \propto t^{1/p}$). The dark energy equation of state during the radiation and matter eras deviates from the Λ CDM value $w_{\text{DE}} = -1$ with the differences $-4s/3$ and $-s$, respectively. For powers satisfying $p \gg p_2$, this deviation tends to be smaller. In fact, taking the limit $p \rightarrow \infty$ in Eq. (13.39), the field ϕ stays constant, so the cosmological dynamics mimics that of the Λ CDM model.

The stability of fixed points (a), (b), (c) is known by perturbing Eqs. (13.46) and (13.47) around them. The eigenvalues of the 2×2 Jacobian matrix for the points (a), (b), (c) are given, respectively, by

$$(a) \quad \mu_1 = 4(1+s), \quad \mu_2 = 1, \quad (13.57)$$

$$(b) \quad \mu_1 = 3(1+s), \quad \mu_2 = -1, \quad (13.58)$$

$$(c) \quad \mu_1 = -3, \quad \mu_2 = -4. \quad (13.59)$$

This means that the de Sitter fixed point (c) is always stable irrespective of the value of s . Provided that $s > -1$ the radiation fixed point (a) is unstable, while the matter point (b) is a saddle. Then, the cosmological trajectory is given by the sequence of the fixed points: (a) $\rightarrow$ (b) $\rightarrow$ (c). The dark energy equation of state

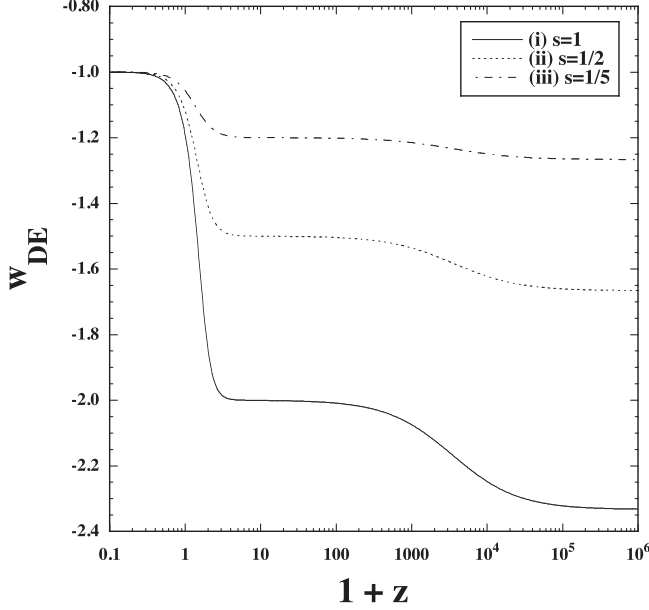


Fig. 13.1. Evolution of w_{DE} versus $1+z$ for the three cases (i) $s = 1$, (ii) $s = 1/2$, and (iii) $s = 1/5$. In each case the initial conditions are chosen to be (i) $\Omega_{\text{DE}} = 1.0 \times 10^{-42}$, $\Omega_r = 0.998$ at $z = 1.7 \times 10^6$, (ii) $\Omega_{\text{DE}} = 1.5 \times 10^{-36}$, $\Omega_r = 0.9996$ at $z = 9.0 \times 10^6$, and (iii) $\Omega_{\text{DE}} = 7.0 \times 10^{-29}$, $\Omega_r = 0.9995$ at $z = 6.9 \times 10^6$. Reproduced from Ref. [4].

evolves as $w_{\text{DE}} = -1 - 4s/3$ (radiation era) $\rightarrow w_{\text{DE}} = -1 - s$ (matter era), and then it finally approaches the de Sitter attractor (c) with $w_{\text{DE}} = -1$. For $s = 1$, the above cosmological trajectory is equivalent to the tracker solution arising for scalar Galileons discussed in Sec. 11.3.4.

In Fig. 13.1, we plot the evolution of w_{DE} for three different values of s . The vector Galileon corresponds to $s = 1$, in which case $w_{\text{DE}} = -2$ during the matter era. This model, which is equivalent to the tracker solution of scalar Galileons, is in tension with the combined observational constraints of SNIa, WMAP, and BAO [16]. However, the models with smaller s can be consistent with the data. The likelihood analysis based on the SNIa, Planck, BAO, and H_0 data showed that the parameter s is constrained to be $s = 0.254^{+0.118}_{-0.097}$ at 95% CL [17]. Hence the Λ CDM model is disfavored over the model with $s > 0$ at 95% CL in current observations.

In the Λ CDM model, the best-fit values of $\Omega_m^{(0)}$ and h constrained by the Planck data are around $\Omega_m^{(0)} \simeq 0.31$ and $h \simeq 0.68$ [18]. These values are in tension with their low-redshift measurements, which generally favor lower $\Omega_m^{(0)}$ and higher h . The model with $s > 0$ can reduce the tension with the shift toward smaller $\Omega_m^{(0)}$ and larger h relative to those in the Λ CDM model. It remains to be seen whether such a property also persists in future high-precision observational data.

13.4. Stability conditions

Let us study the evolution of linear cosmological perturbations on the flat FLRW background and derive theoretically consistent conditions in generalized Proca theories. Since there are two vector propagating DOFs in addition to one scalar mode and two tensor polarizations, we need to discuss the evolution of vector perturbations. In doing so, we consider the perturbed line element in the flat gauge:

$$ds^2 = -(1 + 2\alpha) dt^2 + 2 (\partial_i \chi + V_i) dt dx^i + a^2(t) (\delta_{ij} + h_{ij}) dx^i dx^j, \quad (13.60)$$

where α, χ are scalar metric perturbations, V_i is the vector perturbation satisfying the transverse condition $\partial^i V_i = 0$, and h_{ij} is the tensor perturbation obeying the transverse and traceless conditions $\partial^i h_{ij} = 0$ and $h_i^i = 0$. Compared to the full perturbed line element (6.13), we have the correspondence $A \rightarrow \alpha$, $B \rightarrow a^{-1}\chi$, $S_i \rightarrow -a^{-1}V_i$, $\psi \rightarrow 0$, $E \rightarrow 0$, and $F_i \rightarrow 0$. As we see from Eqs. (6.31), (6.32) and (6.33), the gauge transformation vectors ξ^0, ξ, ζ_i are completely fixed by the gauge choice (13.60).

We also decompose temporal and spatial components of the vector field $A^\mu(t, \mathbf{x})$ into the background and perturbed components as

$$A^0 = \phi(t) + \delta\phi, \quad (13.61)$$

$$A^i = \frac{1}{a^2(t)} \delta^{ij} (\partial_j \chi_V + E_j), \quad (13.62)$$

where the perturbation $\delta\phi$ depends on both time t and spatial position $\mathbf{x}$. The perturbations χ_V and E_j correspond to the intrinsic scalar and vector parts of A_i , respectively. The vector part obeys the transverse condition $\partial^j E_j = 0$.

For the matter sector, we employ the Schutz–Sorkin action given by Eq. (6.203), which is suitable for accommodating vector perturbations. We take into account a single perfect fluid with energy density ρ and pressure P , but it is easy to extend the analysis to the multi-field set-up. The four-dimensional vector field J^μ has the temporal component (6.208) and the spatial vector components (6.209). They contain scalar perturbations $\delta J, \delta j$ and the vector perturbation W_k satisfying the transverse condition $\partial^k W_k = 0$. The perturbed part of the scalar quantity ℓ , which appears in the Schutz–Sorkin action (6.203), is related to the velocity potential $\mathcal{V}$.

The quantities $\mathcal{A}_1, \mathcal{A}_2, \mathcal{B}_1, \mathcal{B}_2$, which are associated with vector perturbations, are chosen as Eq. (6.211). The four velocity u_μ , which is defined by Eq. (6.205), has the spatial vector component $u_i = -\partial_i \mathcal{V} + \mathcal{V}_i$, see Eq. (6.213). The perturbations $\delta \mathcal{A}_i$ are related to the intrinsic vector part $\mathcal{V}_i$, as $\delta \mathcal{A}_i = \rho_{,n} \mathcal{V}_i$. To satisfy the transverse conditions $\partial^i V_i = 0$ and $\partial^i E_i = 0$ for the vector perturbations V_i and E_i in Eqs. (13.60) and (13.62), we take them in the forms $V_i = (V_1(t, z), V_2(t, z), 0)$ and $E_i = (E_1(t, z), E_2(t, z), 0)$ respectively.

In the following, we derive second-order actions of tensor, vector, and scalar perturbations to identify theoretically consistent conditions of generalized Proca theories on the flat FLRW background.

13.4.1. Tensor perturbations

We first expand the action (13.31) up to second order in tensor perturbations. We decompose h_{ij} into the two polarization modes h_+ and $h_\times$ as Eq. (6.153) in terms of polarization tensors e_{ij}^+ and $e_{ij}^\times$ obeying the normalizations (6.154). Then, the second-order action of generalized Proca theories reads [4]

$$S_t^{(2)} = \sum_{\lambda=+,\times} \int dt d^3x a^3 \frac{q_t}{4} \left[\dot{h}_\lambda^2 - \frac{c_t^2}{a^2} (\partial h_\lambda)^2 \right], \quad (13.63)$$

where

$$q_t = 2G_4 - 2\phi^2 G_{4,X} + H\phi^3 G_{5,X}, \quad (13.64)$$

$$c_t^2 = \frac{2G_4 + \phi^2 \dot{\phi} G_{5,X}}{q_T}. \quad (13.65)$$

We require the conditions $q_t > 0$ and $c_t^2 > 0$ to avoid ghosts and Laplacian instabilities of the tensor sector.

13.4.2. Vector perturbations

For vector perturbations, the first process is to expand the Schutz–Sorkin matter action (6.203) that contains intrinsic vector perturbations $W_i, \delta\mathcal{A}_i, \delta\mathcal{B}_i$ and V_i . The resulting second-order action is given by [4]

$$(S_M^{(2)})_v = \int dt d^3x \sum_{i=1}^2 \left[\frac{1}{2a^2 \mathcal{N}_0} \{ \rho_{,n} (W_i^2 + \mathcal{N}_0^2 V_i^2) + \mathcal{N}_0 (2\rho_{,n} V_i W_i - a^3 \rho V_i^2) \} \right. \\ \left. - \mathcal{N}_0 \delta\mathcal{A}_i \delta\mathcal{B}_i - \frac{1}{a^2} W_i \delta\mathcal{A}_i \right], \quad (13.66)$$

where $\mathcal{N}_0$ is the total fluid number defined by Eq. (6.206) (which is constant). Expansion of the action S_{GP} up to second order in vector perturbations does not give rise to the quantities $W_i, \delta\mathcal{A}_i, \delta\mathcal{B}_i$. Hence the equations of motion for these perturbations follow by varying the second-order matter action (13.66) with respect to $W_i, \delta\mathcal{A}_i, \delta\mathcal{B}_i$.

Variation of the action (13.66) with respect to W_i gives

$$W_i = \mathcal{N}_0 (\mathcal{V}_i - V_i), \quad (13.67)$$

where we used the relation $\delta\mathcal{A}_i = \rho_{,n} \mathcal{V}_i$. Substituting this relation into Eq. (13.66) and varying the action in terms of $\delta\mathcal{A}_i$, it follows that

$$\delta\mathcal{A}_i = \rho_{,n} (\mathcal{V}_i - a^2 \delta\mathcal{B}_i), \quad (13.68)$$

and hence $\mathcal{V}_i = V_i - a^2 \delta\mathcal{B}_i$. Variation of the action (13.66) with respect to $\delta\mathcal{B}_i$ leads to the conservation equation

$$\delta\mathcal{A}_i = C_i, \quad (13.69)$$

where C_i ($i = 1, 2$) are constants in time (but they can depend on scales). On using Eqs. (6.206) and (6.207), this relation translates to

$$\frac{\mathcal{N}_0 C_i}{(\rho + P)a^3} = \mathcal{V}_i = V_i - a^2 \delta \dot{\mathcal{B}}_i. \quad (13.70)$$

After integrating out the fields W_i and δA_i , the matter action (13.66) reduces to

$$(S_M^{(2)})_v = \int dt d^3x \sum_{i=1}^2 \frac{a}{2} \left[(\rho + P) \left(V_i - a^2 \delta \dot{\mathcal{B}}_i \right)^2 - \rho V_i^2 \right]. \quad (13.71)$$

The next step is to expand the action S_{GP} up to second order in vector perturbations. In doing so, we define the following combination

$$Z_i = E_i + \phi(t) V_i. \quad (13.72)$$

The perturbation Z_i is equivalent to the intrinsic vector part of A_i by using Eqs. (13.61) and (13.62) with the perturbed line element (13.60). We also introduce the rescaled fields

$$\tilde{V}_i \equiv \frac{V_i}{a}, \quad \tilde{Z}_i \equiv \frac{Z_i}{a}. \quad (13.73)$$

Expanding the action S_{GP} and summing it with the matter part (13.71), the quadratic action of vector perturbations yields [19]

$$\begin{aligned} S_v^{(2)} = \int dt d^3x \sum_{i=1}^2 a^3 \left[\frac{q_v}{2} \dot{\tilde{Z}}_i^2 - \frac{1}{2a^2} \alpha_1 (\partial \tilde{Z}_i)^2 - \frac{1}{2} \alpha_2 \tilde{Z}_i^2 + \frac{q_t}{4a^2} (\partial \tilde{V}_i)^2 \right. \\ \left. + \frac{\phi}{2a^2} (2G_{4,X} - G_{5,X} H \phi) \partial \tilde{V}_i \partial \tilde{Z}_i + \frac{1}{2} (\rho + P) (\tilde{V}_i - a \delta \dot{\mathcal{B}}_i)^2 \right], \end{aligned} \quad (13.74)$$

where

$$q_v = G_{2,F} + 2G_{2,Y} \phi^2 - 4g_5 H \phi + 2G_6 H^2 + 2G_{6,X} H^2 \phi^2, \quad (13.75)$$

$$\alpha_1 = q_v + 2[G_6 \dot{H} - G_{2,Y} \phi^2 - (H\phi - \dot{\phi})(H\phi G_{6,X} - g_5)], \quad (13.76)$$

$$\begin{aligned} \alpha_2 = 2(2G_{4,X} - H\phi G_{5,X}) \dot{H} + (G_{3,X} + 4\phi H G_{4,XX} - G_{5,X} H^2 - \phi^2 G_{5,XX} H^2) \dot{\phi} \\ + 2q_v H^2 + \frac{d}{dt}(q_v H). \end{aligned} \quad (13.77)$$

Varying the action (13.74) with respect to $\tilde{V}_i$ and $\tilde{Z}_i$ in Fourier space, it follows that

$$\frac{q_t}{2} \frac{k^2}{a^2} \tilde{V}_i = -\frac{\mathcal{N}_0 C_i}{a^4} - \frac{\phi}{2} (2G_{4,X} - G_{5,X} H \phi) \frac{k^2}{a^2} \tilde{Z}_i, \quad (13.78)$$

$$\begin{aligned} \ddot{\tilde{Z}}_i + \left(3H + \frac{\dot{q}_v}{q_v} \right) \dot{\tilde{Z}}_i + \left[\frac{\alpha_1}{q_v} + \frac{\phi^2}{2q_v q_t} (2G_{4,X} - G_{5,X} H \phi)^2 \right] \frac{k^2}{a^2} \tilde{Z}_i + \frac{\alpha_2}{q_v} \tilde{Z}_i \\ = -\frac{\phi}{q_v q_t} (2G_{4,X} - G_{5,X} H \phi) \frac{\mathcal{N}_0 C_i}{a^4}, \end{aligned} \quad (13.79)$$

where we used Eq. (13.70). From Eq. (13.78), the vector field $\tilde{V}_i$ does not depend on the time derivative $\dot{\tilde{Z}}_i$, so the kinetic term $q_v \dot{\tilde{Z}}_i^2/2$ in Eq. (13.74) is unchanged after eliminating the contribution of $\tilde{V}_i$ -dependent terms from the action (13.74). As we see from Eq. (13.79), the dynamical vector propagating DOFs are the perturbations $\tilde{Z}_i$, which have two independent modes ($i = 1, 2$) as expected. The vector ghost is absent under the condition

$$q_v > 0. \quad (13.80)$$

In the small-scale limit, the vector propagation speed squared corresponds to the coefficient in front of the $(k^2/a^2)\tilde{Z}_i$ term in Eq. (13.79), such that

$$c_v^2 = 1 + \frac{\phi^2(2G_{4,X} - G_{5,X}H\phi)^2}{2q_t q_v} + \frac{2[G_6\dot{H} - G_{2,Y}\phi^2 - (H\phi - \dot{\phi})(H\phi G_{6,X} - g_5)]}{q_v}. \quad (13.81)$$

To avoid the Laplacian instability of small-scale perturbations, we require that $c_v^2 > 0$. It should be noted that intrinsic vector modes like the contribution Y to $\mathcal{L}_2$, the g_5 -dependent term in $\mathcal{L}_5$, the Lagrangian density $\mathcal{L}_6$ affect both q_v and c_v^2 . From Eq. (13.79), we define the mass squared of dynamical vector fields $\tilde{Z}_i$ as

$$m_v^2 \equiv \frac{\alpha_2}{q_v}. \quad (13.82)$$

Since $\alpha_2 = 2q_v H^2$ on de Sitter solutions (satisfying $\dot{H} = 0$ and $\dot{\phi} = 0$), the mass squared is equivalent to $2H^2$. This means that, even when the mass squared m^2 in the original Proca theory (13.1) is negative, there is no tachyonic instability on de Sitter solutions.

To discuss the evolution of small-scale perturbations deep inside the vector sound horizon ($c_v^2 k^2/a^2 \gg H^2$), we take the limit $k \rightarrow \infty$ in Eq. (13.78) by assuming that the constants C_i are independent of k . Then, it follows that

$$\tilde{V}_i \simeq -\frac{\phi}{q_t} (2G_{4,X} - G_{5,X}H\phi) \tilde{Z}_i. \quad (13.83)$$

On using this relation, the second-order action (13.74) in Fourier space reads

$$S_v^{(2)} \simeq \int dt d^3x \sum_{i=1}^2 \frac{a^3 q_v}{2} \left(\dot{\tilde{Z}}_i^2 + c_v^2 \frac{k^2}{a^2} \tilde{Z}_i^2 \right), \quad (13.84)$$

where we have ignored the mass term $m_v^2 \tilde{Z}_i^2$ relative to $(k^2/a^2)\tilde{Z}_i^2$. This action can be written in the form

$$S_v^{(2)} \simeq \int d\eta d^3x \sum_{i=1}^2 \frac{1}{2} \left[\mathcal{U}_i'^2 + \left(c_v^2 k^2 + \frac{z_v''}{z_v} \right) \mathcal{U}_i^2 \right], \quad (13.85)$$

where a prime represents a derivative with respect to the conformal time $\eta = \int a^{-1} dt$, and

$$\mathcal{U}_i = z_v \tilde{Z}_i, \quad z_v = a\sqrt{q_v}. \quad (13.86)$$

As long as the variation of q_v is not significant such that the conditions $|\dot{q}_v| \lesssim |Hq_v|$ and $|\ddot{q}_v| \lesssim |H^2 q_v|$ are satisfied, we have $c_v^2 k^2 \mathcal{U}_i^2 \gg |(z_v''/z_v) \mathcal{U}_i^2|$ for perturbations deep inside the vector sound horizon. In this case, the equation of motion for $\mathcal{U}_i$ is approximately given by

$$\mathcal{U}_i'' + c_v^2 k^2 \mathcal{U}_i \simeq 0. \quad (13.87)$$

Provided that the frequency $\omega_k = c_v k$ adiabatically changes in time, we obtain the WKB solution in the form

$$\tilde{Z}_i = \frac{\mathcal{U}_i}{z_v} \simeq \frac{1}{a\sqrt{2q_v c_v k}} (\alpha_k e^{-ic_v k \eta} + \beta_k e^{ic_v k \eta}), \quad (13.88)$$

where α_k and β_k are integration constants. Hence, the perturbations $\tilde{Z}_i$ exhibit damped oscillations with decreasing amplitudes.

If the vector field A^μ is responsible for the late-time cosmic acceleration, the quantities $G_{4,X}$ and $G_{5,X}$ in Eq. (13.83) hardly contribute to the background cosmological dynamics during the radiation and matter eras, so the perturbations $\tilde{V}_i$ are suppressed to be small. The solution to the dynamical vector field $\tilde{Z}_i$ is approximately given by Eq. (13.88) from the vector sound horizon entry ($c_v^2 k^2/a^2 = H^2$) to today. The vector perturbations $\tilde{Z}_i$ decay for q_v and c_v^2 adiabatically changing in time [19].

In Ref. [20], the authors studied the evolution of a spatial component $v(t)$ of the massive vector field on an anisotropic cosmological background. It was shown that, during the radiation era, the spatial component works as a dark radiation with the equation of state close to $1/3$. After the onset of the matter-dominated epoch, it decays toward the asymptotic value $v = 0$ at the de Sitter fixed point. This is consistent with the above result where the spatial component has been treated as a perturbation on the isotropic FLRW background. The ratio Σ/H between the anisotropic expansion rate Σ and the isotropic expansion rate H also decreases after the radiation era.

13.4.3. Scalar perturbations

In Sec. 6.9, we derived the second-order Schutz–Sorkin action of scalar perturbations in the form (6.223) for the metric (6.218). For the metric (13.60) we just need to

replace $\Psi \rightarrow \alpha$ and $\Phi \rightarrow 0$ in Eq. (6.223), so the action in the matter sector yields

$$S_M^{(2)} = \int dt d^3x a^3 \left\{ \left(\dot{\mathcal{V}} - 3H c_M^2 \mathcal{V} - \alpha \right) \delta\rho - \frac{c_M^2 \delta\rho^2}{2n_0\rho_{,n}} - \frac{n_0\rho_{,n}}{2a^2} [(\partial\mathcal{V})^2 + 2\partial\mathcal{V}\partial\chi] \right. \\ \left. + \frac{1}{2}\rho\alpha^2 - \frac{\rho}{2a^2}(\partial\chi)^2 \right\}, \quad (13.89)$$

where $\delta\rho = \rho_{,n}\delta J/a^3$ is the matter density perturbation and $c_M^2 = n_0\rho_{,nn}/\rho_{,n}$ is the matter propagation speed squared.

It is also convenient to introduce the following combination

$$\psi = \chi_V + \phi(t)\chi. \quad (13.90)$$

From Eqs. (13.61) and (13.62) the scalar part of A_i corresponds to $\partial_i\psi$. Expanding the action S_{GP} up to second order in scalar perturbations and then taking the sum with Eq. (13.89), the total second-order action for scalar perturbations reads [4]

$$S_S^{(2)} = \int dt d^3x a^3 \left\{ -\frac{n_0\rho_{,n}}{2} \frac{(\partial\mathcal{V})^2}{a^2} + \left[n_0\rho_{,n} \frac{\partial^2\chi}{a^2} - \delta\rho - 3H(1+c_M^2)\delta\rho \right] \mathcal{V} \right. \\ - \left[(3Hz_1 - 2z_4) \frac{\delta\phi}{\phi} - z_3 \frac{\partial^2(\delta\phi)}{a^2\phi} - z_3 \frac{\partial^2\dot{\psi}}{a^2\phi} + z_6 \frac{\partial^2\psi}{a^2} \right] \alpha - z_3 \frac{(\partial\alpha)^2}{a^2} + z_4\alpha^2 \\ - \frac{z_3}{4} \frac{(\partial\delta\phi)^2}{a^2\phi^2} + z_5 \frac{(\delta\phi)^2}{\phi^2} - \left[\frac{(z_6\phi + z_2)\psi}{2} - \frac{z_3}{2}\dot{\psi} \right] \frac{\partial^2(\delta\phi)}{a^2\phi^2} - \frac{z_3}{4\phi^2} \frac{(\partial\dot{\psi})^2}{a^2} \\ \left. + \frac{z_7}{2} \frac{(\partial\psi)^2}{a^2} + \left(z_1\alpha + \frac{z_2\delta\phi}{\phi} \right) \frac{\partial^2\chi}{a^2} - \alpha\delta\rho - \frac{c_M^2}{2n_0\rho_{,n}}(\delta\rho)^2 \right\}, \quad (13.91)$$

where

$$z_1 = H^2\phi^3(G_{5,X} + \phi^2G_{5,XX}) - 4H(G_4 + \phi^4G_{4,XX}) - \phi^3G_{3,X}, \quad (13.92)$$

$$z_2 = z_1 + 2Hq_t, \quad (13.93)$$

$$z_3 = -2\phi^2q_v, \quad (13.94)$$

$$z_4 = \frac{1}{2}H^3\phi^3(9G_{5,X} - \phi^4G_{5,XXX}) - 3H^2(2G_4 + 2\phi^2G_{4,X} + \phi^4G_{4,XX}) \\ - \phi^6G_{4,XXX} - \frac{3}{2}H\phi^3(G_{3,X} - \phi^2G_{3,XX}) + \frac{1}{2}\phi^4G_{2,XX}, \quad (13.95)$$

$$z_5 = z_4 - \frac{3}{2}H(z_1 + z_2), \quad (13.96)$$

$$z_6 = -\phi[H^2\phi(G_{5,X} - \phi^2G_{5,XX}) - 4H(G_{4,X} - \phi^2G_{4,XX}) + \phi G_{3,X}], \quad (13.97)$$

$$z_7 = 2(H\phi G_{5,X} - 2G_{4,X})\dot{H} + [H^2(G_{5,X} + \phi^2G_{5,XX}) \\ - 4H\phi G_{4,XX} - G_{3,X}]\dot{\phi}. \quad (13.98)$$

The terms containing $G_{2,F}, G_{2,Y}, g_5, G_6, G_{6,X}$ arise only in the coefficient z_3 , so the functions $g_5(X), G_6(X)$ as well as $G_2(F, Y)$ lead to modifications to the quadratic action (13.91) through the change of q_v .

Varying the action (13.91) with respect to $\alpha, \chi, \delta\phi, \mathcal{V}, \partial\psi, \delta\rho$ in Fourier space, respectively, we obtain the following equations of motion

$$\delta\rho - 2z_4\alpha + (3Hz_1 - 2z_4) \frac{\delta\phi}{\phi} + \frac{k^2}{a^2} (\mathcal{V} + z_1\chi - z_6\psi) = 0, \quad (13.99)$$

$$(\rho + P) \mathcal{V} + z_1\alpha + \frac{z_2}{\phi} \delta\phi = 0, \quad (13.100)$$

$$(3Hz_1 - 2z_4) \alpha - 2z_5 \frac{\delta\phi}{\phi} + \frac{k^2}{a^2} \left[\frac{1}{2} \mathcal{V} + z_2\chi - \frac{1}{2} \left(\frac{z_2}{\phi} + z_6 \right) \psi \right] = 0, \quad (13.101)$$

$$\dot{\delta\rho} + 3H (1 + c_M^2) \delta\rho + \frac{k^2}{a^2} (\rho + P) (\chi + \mathcal{V}) = 0, \quad (13.102)$$

$$\dot{\mathcal{V}} + \left(H - \frac{\dot{\phi}}{\phi} \right) \mathcal{V} + 2\phi (z_6\alpha + z_7\psi) + \left(\frac{z_2}{\phi} + z_6 \right) \delta\phi = 0, \quad (13.103)$$

$$\dot{\mathcal{V}} - 3Hc_M^2 \mathcal{V} - c_M^2 \frac{\delta\rho}{\rho + P} - \alpha = 0, \quad (13.104)$$

where

$$\mathcal{V} \equiv \frac{z_3}{\phi} \left(\dot{\psi} + \delta\phi + 2\alpha\phi \right). \quad (13.105)$$

The fields $\alpha, \chi, \delta\phi, \mathcal{V}$ do not correspond to dynamical fields, which can be eliminated from the action (13.91) by using Eqs. (13.99)–(13.102). After integrations by parts, the action (13.91) is expressed in terms of two dynamical fields ψ and $\delta\rho$ as

$$S_S^{(2)} = \int dt d^3x a^3 \left(\dot{\vec{\chi}}^t \mathbf{K} \dot{\vec{\chi}} + \frac{k^2}{a^2} \vec{\chi}^t \mathbf{G} \vec{\chi} - \vec{\chi}^t \mathbf{M} \vec{\chi} - \vec{\chi}^t \mathbf{B} \dot{\vec{\chi}} \right), \quad (13.106)$$

where $\mathbf{K}, \mathbf{G}, \mathbf{M}, \mathbf{B}$ are 2×2 matrices, and the vector field $\vec{\chi}$ is defined by

$$\vec{\chi}^t = (\psi, \delta\rho/k). \quad (13.107)$$

The matrix $\mathbf{M}$, which is associated with masses of two scalar modes, does not contain the k^2/a^2 term. In the small-scale limit ($k \rightarrow \infty$), the second term on the right hand side of Eq. (13.106) dominates over the third and fourth terms.

The matrix $\mathbf{K}$ is related to the kinetic terms of two scalar perturbations ψ and $\delta\rho$. As long as two eigenvalues of $\mathbf{K}$ are positive, there are no scalar ghosts. The

no-ghost condition for the matter perturbation $\delta\rho$ is trivially satisfied for $\rho + P > 0$. Another no-ghost condition associated with the perturbation ψ is given by

$$Q_s = \frac{a^3 H^2 q_t q_s}{\phi^2 (z_1 - 2z_2)^2} > 0, \quad (13.108)$$

where

$$q_s \equiv 3z_1^2 + 4q_t z_4. \quad (13.109)$$

Provided that the tensor ghost is absent ($q_t > 0$), the scalar ghost does appear for $q_s > 0$.

In the $k \rightarrow \infty$ limit, the action (13.106) leads to the dispersion relation $\det(c_s^2 \mathbf{K} - \mathbf{G}) = 0$, where c_s corresponds to the sound speed related to a frequency ω as $\omega^2 = c_s^2 k^2 / a^2$. One of the solutions to this equation is the matter propagation speed squared c_M^2 . Another is the propagation speed squared of the perturbation ψ , which is given by

$$\begin{aligned} c_s^2 = \frac{1}{\Delta} \bigg\{ & 2z_2^2 z_3 (\rho + P) - z_3 (z_1 - 2z_2) [z_1 z_2 + \phi (z_1 - 2z_2) z_6] \left(\dot{\phi} / \phi - H \right) \\ & - z_3 (2z_2^2 \dot{z}_1 - z_1^2 \dot{z}_2) + \phi (z_1 - 2z_2)^2 [z_3 \dot{z}_6 + \phi (2z_3 z_7 + z_6^2)] \\ & + z_1 z_2 [z_1 z_2 + (z_1 - 2z_2)(2z_6 \phi - z_3 \dot{\phi} / \phi)] \bigg\}, \end{aligned} \quad (13.110)$$

where

$$\Delta \equiv 8H^2 \phi^2 q_t q_v q_s. \quad (13.111)$$

The Laplacian instability of scalar perturbations is absent for $c_s^2 > 0$. Under the three no-ghost conditions $q_t > 0$, $q_v > 0$, and $q_s > 0$, the condition $c_s^2 > 0$ is satisfied as long as the numerator of Eq. (13.110) is positive. In the presence of multiple fluids, we only need to add each energy density ρ_i and pressure P_i to ρ and P respectively.

In summary, the number of propagating degrees of freedom is five (two tensors, two vectors, one scalar) besides a scalar mode from the matter sector. Three of them (two vectors and one scalar) originate from the massive vector field. We require that the six quantities q_t, q_v, q_s and c_t^2, c_v^2, c_s^2 are positive for the theoretical consistency of generalized Proca theories.

13.5. Effective gravitational couplings

To discuss observational signatures of generalized Proca theories, we derive the effective gravitational coupling with a non-relativistic perfect fluid satisfying $P = 0$ and $c_M^2 = 0$. We introduce the gauge-invariant density contrast as Eq. (12.28), i.e.,

$\delta_m \equiv \delta\rho/\rho + 3H\mathcal{V}$ for $w = 0$. Taking the time derivative of Eq. (13.102) and using Eq. (13.104), we obtain

$$\ddot{\delta}_m + 2H\dot{\delta}_m + \frac{k^2}{a^2}\Psi = 3\left(\ddot{I} + 2H\dot{I}\right), \quad (13.112)$$

where $I \equiv H\mathcal{V}$, and Ψ is the gauge-invariant gravitational potential given by Eq. (6.63), i.e.,

$$\Psi = \alpha + \dot{\chi}, \quad (13.113)$$

for the perturbed line element (13.60) in the flat gauge. Another gauge-invariant potential (6.64) reads

$$\Phi = H\chi. \quad (13.114)$$

As we see below, it is possible to derive analytic expressions of Ψ and Φ under the quasi-static approximation on sub-horizon scales mentioned in Sec. 12.2. Under this approximation, the dominant terms to perturbation equations are those containing k^2/a^2 and $\delta\rho$. Then, Eqs. (13.99) and (13.101) reduce, respectively, to

$$\delta\rho \simeq -\frac{k^2}{a^2}(\mathcal{Y} + z_1\chi - z_6\psi), \quad (13.115)$$

$$\mathcal{Y} \simeq \left(\frac{z_2}{\phi} + z_6\right)\psi - 2z_2\chi. \quad (13.116)$$

Substituting Eq. (13.116) into Eq. (13.115), we obtain

$$\delta\rho \simeq -\frac{k^2}{a^2}\left(\frac{z_1 - 2z_2}{H}\Phi + \frac{z_2}{\phi}\psi\right), \quad (13.117)$$

where we used Eq. (13.114).

From Eqs. (13.100) and (13.102), the perturbation $\mathcal{V}$ can be eliminated to give

$$\dot{\delta}\rho + 3H\delta\rho + \frac{k^2}{a^2}\left(\rho\chi - z_1\alpha - \frac{z_2}{\phi}\delta\phi\right) = 0. \quad (13.118)$$

Taking the time derivative of Eq. (13.117) and using Eqs. (13.118) and (13.105), we can remove $\dot{\delta}\rho$ and $\delta\rho$ as well as the $\dot{\psi}$ term. Since the perturbation $\alpha + \dot{\chi}$ can be expressed in terms of Ψ , it follows that

$$\phi^2(z_1 - 2z_2)z_3\Psi + \mu_1\Phi + \mu_2\psi \simeq 0, \quad (13.119)$$

where

$$\mu_1 = \frac{\phi^2}{H}[(\dot{z}_1 - 2\dot{z}_2 + Hz_1 - \rho)z_3 - 2z_2(z_2 + Hz_3)], \quad (13.120)$$

$$\mu_2 = \phi(z_2^2 + Hz_2z_3 + \dot{z}_2z_3) + z_2(z_6\phi^2 - z_3\dot{\phi}). \quad (13.121)$$

After differentiating Eq. (13.116) with respect to t , it is possible to eliminate $\dot{\mathcal{Y}}$ and $\mathcal{Y}$ terms in Eq. (13.103), such that

$$2\phi^2 z_2 \Psi + \mu_3 \Phi + \mu_4 \psi \simeq 0, \quad (13.122)$$

where

$$\mu_3 \equiv \frac{2\phi}{H z_3} \mu_2, \quad (13.123)$$

$$\begin{aligned} \mu_4 \equiv & -\frac{1}{z_3} \left[\phi^3 (z_6^2 + 2z_3 z_7) + \phi^2 (2z_2 z_6 + H z_3 z_6 + z_3 \dot{z}_6) \right. \\ & \left. + \phi \left\{ z_2^2 + H z_2 z_3 + z_3 (\dot{z}_2 - \dot{\phi} z_6) \right\} - 2\dot{\phi} z_2 z_3 \right]. \end{aligned} \quad (13.124)$$

Now, we can solve Eqs. (13.117), (13.119), (13.122) for two gauge-invariant potentials Ψ, Φ and the dynamical field ψ . In doing so, we employ the approximation $\delta_m \simeq \delta\rho/\rho$, whose validity is ensured for perturbations deep inside the sound horizon. Then, it follows that

$$\Psi \simeq -\frac{H(\mu_2 \mu_3 - \mu_1 \mu_4)}{\phi \mu_5} \frac{a^2}{k^2} \rho \delta_m, \quad (13.125)$$

$$\Phi \simeq \frac{\phi H [2z_2 \mu_2 - (z_1 - 2z_2) z_3 \mu_4]}{\mu_5} \frac{a^2}{k^2} \rho \delta_m, \quad (13.126)$$

$$\psi \simeq \frac{\phi H [z_1 z_3 \mu_3 - 2z_2 (\mu_1 + z_3 \mu_3)]}{\mu_5} \frac{a^2}{k^2} \rho \delta_m, \quad (13.127)$$

where

$$\mu_5 \equiv (z_1 - 2z_2) [\phi (z_1 - 2z_2) z_3 \mu_4 - 2\phi z_2 \mu_2] + H z_2 [2z_2 (\mu_1 + z_3 \mu_3) - z_1 z_3 \mu_3]. \quad (13.128)$$

Neglecting the right hand side of Eq. (13.112) relative to the left hand side of it under the quasi-static approximation on sub-horizon scales and using Eq. (13.125), we obtain [19]

$$\ddot{\delta}_m + 2H\dot{\delta}_m - 4\pi G_{\text{eff}} \rho \delta_m \simeq 0, \quad (13.129)$$

where

$$G_{\text{eff}} = \frac{H(\mu_2 \mu_3 - \mu_1 \mu_4)}{4\pi \phi \mu_5}. \quad (13.130)$$

From Eqs. (13.125) and (13.126), the gravitational slip parameter $\eta = -\Phi/\Psi$ reads

$$\eta = \frac{\phi^2 [2z_2 \mu_2 - (z_1 - 2z_2) z_3 \mu_4]}{\mu_2 \mu_3 - \mu_1 \mu_4}. \quad (13.131)$$

As in the case of Horndeski theories, it is convenient to rewrite Eqs. (13.130) and (13.131) in terms of physical quantities like q_s and c_s^2 associated with no-ghost and

stability conditions. In doing so, we first substitute the relations $z_1 = z_2 - 2Hq_t$ and $z_3 = -2\phi^2 q_v$ into Eq. (13.130). From the definitions of z_1 , q_t , and z_6 given by Eqs. (13.92), (13.64) and (13.97), respectively, we can express $G_{3,X}$, G_4 , $G_{4,X}$ in terms of z_2 , q_t , z_6 and derivatives $G_{4,XX}$, $G_{5,X}$, $G_{5,XX}$. On using these relations with the background equations (13.35)–(13.36), it follows that

$$\rho + P = -2q_t \dot{H} - \frac{\dot{\phi}}{\phi} z_2, \quad (13.132)$$

$$z_7 = \frac{1}{2H\phi^3} \left[(z_2 - z_6\phi) \dot{H}\phi + (z_2 + z_6\phi) H\dot{\phi} \right], \quad (13.133)$$

where we have not omitted the pressure P .

After substituting the relations (13.132) and (13.133) into Eq. (13.110), we can express $\dot{z}_6$ in the expression of G_{eff} with respect to c_s^2 . The resulting effective gravitational coupling G_{eff} contains derivative terms $\dot{H}$ and $\dot{\phi}$. Differentiating Eq. (13.38) with respect to t , combining it with Eq. (13.36), and eliminating G_2 and $G_{2,X}$ on account of Eqs. (13.35) and (13.36), the derivative terms $\dot{H}$ and $\dot{\phi}$ can be expressed in terms of z_1 , q_t , and z_4 . Employing the relation (13.109) to express z_4 with respect to q_s , we obtain

$$\dot{H} = \frac{3z_2^2 - q_s}{2q_t q_s} (\rho + P), \quad (13.134)$$

$$\dot{\phi} = -\frac{3z_2\phi}{q_s} (\rho + P). \quad (13.135)$$

After setting $P = 0$ in Eqs. (13.130) and (13.131), it follows that

$$G_{\text{eff}} = \frac{\xi_2 + \xi_3}{\xi_1}, \quad (13.136)$$

$$\eta = \frac{\xi_4}{\xi_2 + \xi_3}, \quad (13.137)$$

where

$$\xi_1 = 4\pi\phi^2 (z_2 + 2Hq_t)^2, \quad (13.138)$$

$$\xi_2 = [H(z_2 + 2Hq_t) - \dot{z}_1 + 2\dot{z}_2 + \rho] \phi^2 - \frac{z_2^2}{q_v}, \quad (13.139)$$

$$\begin{aligned} \xi_3 = & \frac{1}{8H^2\phi^2 q_s^3 q_t c_s^2} \left[2\phi^2 \{q_s[z_2\dot{z}_1 - (z_2 - 2Hq_t)\dot{z}_2] + \rho z_2[3z_2(z_2 + 2Hq_t) - q_s]\} \right. \\ & \left. + \frac{q_s}{q_v} z_2 \{z_2(z_2 - 2Hq_t) - z_6\phi(z_2 + 2Hq_t)\} \right]^2, \end{aligned} \quad (13.140)$$

$$\begin{aligned} \xi_4 = & \frac{z_2 + 2Hq_t}{4Hq_s^2 q_v q_t c_s^2} \left[4H^2\phi^2 q_s^2 q_v q_t c_s^2 + 2\phi^2 q_s q_v z_2 \dot{z}_2 (z_2 - 2Hq_t) + z_2^2 \{\phi q_s z_6 (z_2 + 2Hq_t) \right. \\ & \left. - z_2 q_s (z_2 - 2Hq_t) - 2\phi^2 q_s q_v \dot{z}_1 + 2\phi^2 q_v [q_s - 3z_2(z_2 + 2Hq_t)] \rho \} \right]. \end{aligned} \quad (13.141)$$

For the models in which the condition

$$z_2 = -\phi^2 [\phi G_{3,X} + 4H(G_{4,X} + \phi^2 G_{4,XX}) - H^2 \phi(3G_{5,X} + \phi^2 G_{5,XX})] \neq 0 \quad (13.142)$$

is satisfied, the $1/q_v$ -dependent terms in ξ_2 and ξ_3 do not vanish. If the functions $G_{3,4,5}$ do not have any X dependence, then $z_2 = 0$ and hence G_{eff} is not affected by the term $1/q_v$. In such models we have $z_1 = -4HG_4$ and $q_t = 2G_4$ with constant G_4 , so the quantities (13.138)–(13.141) reduce, respectively, to $\xi_1 = 64\pi G_4^2 H^2 \phi^2$, $\xi_2 = (4G_4 H^2 + 4G_4 \dot{H} + \rho)\phi^2$, $\xi_3 = 0$, and $\xi_4 = 4G_4 H^2 \phi^2$. The relation $4G_4 \dot{H} = -\rho$ follows from the background Eqs. (13.35)–(13.37), so we obtain $G_{\text{eff}} = 1/(16\pi G_4)$ and $\eta = 1$. Since GR corresponds to $G_4 = 1/(16\pi G)$, the effective gravitational coupling reduces to G .

In the following, we consider the case $z_2 \neq 0$. Under the theoretically consistent conditions $q_s > 0$, $q_t > 0$, and $c_s^2 > 0$, it follows that $\xi_3 > 0$. Since ξ_1 is also positive, existence of the term ξ_3/ξ_1 in Eq. (13.136) increases the gravitational attraction. In the expression of ξ_2 there is the term $-z_2^2/q_v$ sourced by the vector sector, which is negative under the no-ghost condition $q_v > 0$. Hence this term works to suppress the gravitational attraction for q_v close to 0. This suggests that it may be possible to realize G_{eff} smaller than the Newton gravitational constant G . The necessary condition for realizing $G_{\text{eff}} < G$ is given by $\xi_2/\xi_1 < G$, i.e.,

$$\phi^2 [(z_2 + 2Hq_t) \{H - 4\pi G(z_2 + 2Hq_t)\} - \dot{z}_1 + 2\dot{z}_2 + \rho] < \frac{z_2^2}{q_v}. \quad (13.143)$$

For the function G_2 containing the standard Maxwell term F , i.e., $G_2 = F + g_2(X, F, Y)$, we have

$$q_v = 1 + g_{2,F} + 2g_{2,Y}\phi^2 - 4g_5 H\phi + 2G_6 H^2 + 2G_{6,X} H^2 \phi^2. \quad (13.144)$$

Existence of the functions $g_2(F, Y)$, g_5 , G_6 allows the possibility for reducing q_v from 1, in which case it is easier to satisfy the condition (13.143). In scalar–tensor Horndeski theories the necessary condition for realizing weak gravity is given by $c_t^2 M_{\text{pl}}^2/(4Q_t) < 1$, whose condition depends only on quantities associated with tensor perturbations. On the other hand, the condition (13.143) depends on both vector and tensor perturbations, so the generalized Proca theory offers a more flexible possibility for the realization of weak gravity. We caution, however, that the condition (13.143) is not sufficient to realize $G_{\text{eff}} < G$ due to the existence of the positive term ξ_3/ξ_1 . In doing so, we need to evaluate the three quantities ξ_1 , ξ_2 , and ξ_3 for given models.

13.6. Observational signatures in large-scale structures

We will study observational signatures of generalized Proca theories associated with the measurement of large-scale structures. For concreteness, we consider the

extended version of power-law functions (13.40), i.e.,

$$\begin{aligned} G_2 &= b_2 X^{p_2} + [1 + g_2(X)] F, & G_3 &= b_3 X^{p_3}, & G_4 &= \frac{1}{16\pi G} + b_4 X^{p_4}, \\ G_5 &= b_5 X^{p_5}, & G_6 &= b_6 X^{p_6}, & g_5 &= \tilde{b}_5 X^{q_5}, \end{aligned} \quad (13.145)$$

where $G = (8\pi M_{\text{pl}}^2)^{-1}$ is the gravitational constant, $b_{2,3,4,5,6}$, $p_{2,3,4,5,6}$, $\tilde{b}_5$, q_5 are constants, and $g_2(X)$ is an arbitrary function of X with $g_2(0) = 0$. The quantity F vanishes at the background level. Moreover the functions G_6 and g_5 do not appear in Eqs. (13.35)–(13.37), so the background cosmological dynamics is exactly the same as that without those terms. In particular, for the powers $p_{3,4,5}$ given by Eq. (13.41), the temporal vector component ϕ evolves as Eq. (13.39). In the following, we consider the model (13.145) with the powers (13.41).

As we discussed in Sec. 13.5, the existence of the vector mode affects the effective gravitational coupling associated with matter density perturbations. For the model (13.145), the quantity q_v is

$$q_v = 1 + g_2 - 4\tilde{b}_5 X^{q_5} H\phi + 2b_6(1 + 2p_6)H^2 X^{p_6}, \quad (13.146)$$

which is required to be positive to avoid the vector ghost. Due to the property (13.39) the last term of Eq. (13.146) is proportional to $\phi^{2(p_6-p)}$, so it is constant for $p_6 = p$. Depending on the sign of the term $2b_6(1 + 2p_6)$, q_v is either larger or smaller than 1. In what follows, we focus on the constant q_v model characterized by

$$p_6 = p, \quad g_2 = 0, \quad \tilde{b}_5 = 0. \quad (13.147)$$

We can express the quantities z_2 and q_t as

$$z_2 = -\frac{2^{1-p_2/2}}{\sqrt{24\pi G}} p_2 \phi^{p_2} \sqrt{b_2 y} [1 + 6\beta_4(1 - 2p_2 - 2p) + 2\beta_5(3p + 2p_2)], \quad (13.148)$$

$$q_t = \frac{1}{8\pi G} \left[1 + 6\beta_4 p_2 \left(\frac{1}{p_2 + p} - 2 \right) y + 6\beta_5 p_2 y \right], \quad (13.149)$$

where y and β_i are given by Eq. (13.42). Since Ω_{DE} and y approach 0 in the asymptotic past, it follows that $z_2 \rightarrow 0$ and $q_t \rightarrow 1/(8\pi G)$. In the early matter era the approximate background equation of motion $\dot{H} \simeq -4\pi G\rho$ holds, so that the quantities ξ_i in Eqs. (13.138)–(13.141) approximately reduce to $\xi_1 \simeq H^2 \phi^2/(4\pi G^2)$, $\xi_2 \simeq H^2 \phi^2/(4\pi G)$, $\xi_3 \simeq 0$, and $\xi_4 \simeq H^2 \phi^2/(4\pi G)$, respectively. In this epoch the effective gravitational coupling (13.136) and the slip parameter (13.137) are close to G and 1, respectively.

The quantity z_2 starts to be away from 0 around from the end of the matter era, so there is the deviation of G_{eff} from G . On the de Sitter fixed point satisfying

$\dot{\phi} = 0$ and $\dot{H} = 0$, Eq. (13.136) reduces to

$$\frac{G_{\text{eff}}}{G} = \frac{(p + p_2)[q_v u^2 - 2p_2 y \{1 - 6\beta_4(2p + 2p_2 - 3) + 2\beta_5(3p + 2p_2 - 3)\}]}{\mathcal{F}}, \quad (13.150)$$

where $u = \sqrt{8\pi G}\phi$, and

$$\begin{aligned} \mathcal{F} = & q_v u^2 [p + p_2 + 6\beta_4 p_2 y + p_2(p + p_2) \{1 - 6\beta_4(1 + 2p + 2p_2) \\ & + 2\beta_5(3 + 3p + 2p_2)\} y] + 2p_2 y [(p + p_2) \{-1 + 6\beta_4(2p + 2p_2 - 3) \\ & + \beta_5(6 - 6p - 4p_2)\} + 6p_2 \{18\beta_4^2(2p + 2p_2 - 1) \\ & - \beta_4[1 + \beta_5(30p + 28p_2 - 6)] + 6\beta_5^2(p + p_2)\} y]. \end{aligned} \quad (13.151)$$

The effective gravitational coupling at the de Sitter point depends on $q_v u^2$, y as well as the model parameters p, p_2, β_4, β_5 .

In the top panel of Fig. 13.2 the evolution of G_{eff}/G is plotted for $p_2 = 1/2$, $p = p_6 = 5/2$, $b_2 = -m^2(8\pi G)^{p_2-1}$ (with $m^2 > 0$), $\beta_4 = 10^{-4}$, $\beta_5 = 0.052$, and $\lambda \equiv u^p H/m = 1$ with five different values of q_v . These model parameters are chosen to satisfy the six conditions $q_t > 0$, $q_v > 0$, $q_s > 0$, $c_t^2 > 0$, $c_v^2 > 0$, $c_s^2 > 0$ from the radiation era to the de Sitter attractor. Note that this is just one example consistent with no-ghost and stability conditions. There are other model parameter spaces in which the above six conditions are consistently satisfied.

The effective gravitational coupling is close to G during the early matter era in all cases shown in Fig. 13.2, but the late-time evolution of G_{eff} depends on the values of q_v . For the model parameters used in Fig. 13.2, we have $y = -0.906$ and $u = 1.252$ at the de Sitter attractor. From the analytic estimation (13.150), the effective gravitational coupling at the de Sitter fixed point decreases for smaller q_v , e.g., $G_{\text{eff}}/G = 1.503$ for $q_v = 0.5$ and $G_{\text{eff}}/G = 0.974$ for $q_v = 0.001$. Thus, it is possible to realize G_{eff} smaller than G for q_v close to 0.

By computing the quantities ξ_1, ξ_2, ξ_3 defined by Eqs. (13.138)–(13.140) numerically, we find that the contribution ξ_2/ξ_1 to G_{eff} is negative at low redshifts for the model parameters used in Fig. 13.2. This is overwhelmed by the positive term ξ_3/ξ_1 in G_{eff} , such that G_{eff} is positive. Thus the necessary condition (13.143) for realizing weak gravity is satisfied for all the cases shown in Fig. 13.2, but the effect of the ξ_3/ξ_1 term is different depending on the values of q_v .

In the bottom panel of Fig. 13.2, we plot the evolution of $f\sigma_8$ for several different values of q_v with the comoving wave number $k = 230a_0H_0$, where $f \equiv \dot{\delta}_m/(H\delta_m)$ is the growth rate of matter perturbations. We have confirmed that the full numerical solutions to Eqs. (13.99)–(13.104) exhibit very good agreement with those derived under the quasi-approximation on sub-horizon scales explained in Sec. 13.5. As we see in Fig. 13.2, the theoretical values of $f\sigma_8$ at low redshifts get smaller for decreasing q_v . This reflects the fact that G_{eff} at the de Sitter attractor decreases for q_v closer to +0.

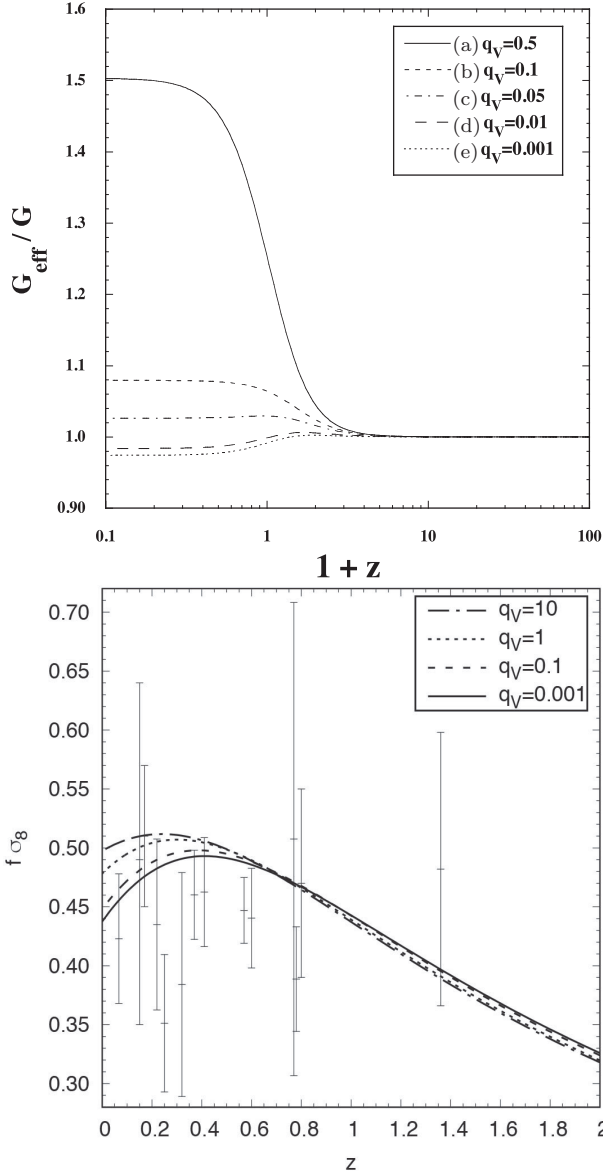


Fig. 13.2. (Top) Evolution of G_{eff}/G versus $1+z$ ($= a_0/a$) for the model parameters $p_2 = 1/2$, $p = p_6 = 5/2$, $g_2 = 0$, $\tilde{b}_5 = 0$, $\beta_4 = 10^{-4}$, $\beta_5 = 0.052$, $\lambda = 1$ with $q_V = 0.5, 0.1, 0.05, 0.01, 0.001$ (from top to bottom). The present epoch (the redshift $z = 0$) corresponds to $\Omega_{\text{DE}} = 0.68$. (Bottom) Evolution of $f\sigma_8$ versus z for the same model parameters as those used in the top panel with $q_V = 10, 1, 0.1, 0.001$. The initial conditions of perturbations are chosen to match those under the sub-horizon approximation with the comoving wave number $k = 230a_0H_0$ and $\sigma_8(z=0) = 0.82$. The black points with error bars show the bounds of $f\sigma_8$ constrained from the data of RSD measurements. Reproduced from Ref. [19].

In the bottom panel of Fig. 13.2, we also show observational data constrained from the RSD measurements. The present values of σ_8 and Ω_{DE} are chosen, respectively, as $\sigma_8(z=0) = 0.82$ and $\Omega_{\text{DE}}^{(0)} = 0.68$, which correspond to the best-fit values of the Planck CMB observations [18]. The theoretical prediction is in tension with some of the RSD data, but this property also persists in the Λ CDM model for $\sigma_8(z=0)$ and $\Omega_{\text{DE}}^{(0)}$ constrained from Planck observations. This tension reduces for smaller $\sigma_8(z=0)$ and larger $\Omega_{\text{DE}}^{(0)}$ constrained from the WMAP data, see e.g., Fig. 12.1. The present RSD data are not sufficiently accurate to place tight constraints on model parameters. It is however interesting to note that generalized Proca theories allow the possibility for reducing G_{eff} due to the existence of the vector mode. In scalar–tensor Horndeski theories, it is generally difficult to realize $G_{\text{eff}} < G$, unless the quantities associated with tensor perturbations are substantially modified from those in GR. Thus, there is a possibility for distinguishing between generalized Proca theories and Horndeski theories from the cosmic growth history.

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Chapter 14

Screening Mechanisms of Fifth Forces

In modified gravity theories, the breaking of gauge symmetry in GR gives rise to propagating scalar or vector degrees of freedom. Since this mediates the propagation of extra forces coupled to non-relativistic matter, we need some screening mechanism of such fifth forces for the compatibility with local gravity experiments in the solar system. There are two representative mechanisms for suppressing the propagation of fifth forces in local regions of the Universe: (i) chameleon mechanism, and (ii) Vainshtein mechanism.

The chameleon mechanism [1, 2] can be at work for a scalar field whose effective mass is different depending on matter densities in the surrounding environment. If the effective mass is sufficiently large in regions of the high density, it is possible to suppress the coupling between the field and non-relativistic matter by having a thin-shell inside a spherically symmetric body. Representative models in which the chameleon mechanism can be at work are $f(R)$ gravity and Brans–Dicke theories in the presence of a scalar potential.

The Vainshtein mechanism [3] can work for a scalar or a vector field with derivative self interactions. Non-linear derivative interactions like those appearing for covariant Galileons, e.g., $X\Box\phi$, can lead to the suppression of fifth forces within a radius (so-called Vainshtein radius) much larger than the solar-system scale.

In this chapter, we review the basics of screening mechanisms and apply them to concrete modified gravity theories. We also study constraints on model parameters from local gravity experiments in the solar system.

14.1. Chameleon mechanism

In Sec. 10.3, we studied a coupled quintessence scenario in which a canonical scalar field ϕ interacts with non-relativistic matter with a coupling of the form (10.112). In the presence of a scalar potential $V(\phi)$, the action of such a coupled quintessence

model is given by Eq. (10.113). In principle, we can consider a more general model in which the couplings between the field and matter are different depending on matter species. Indeed, this is the starting point of the original chameleon model advocated in Refs. [1, 2].

As we showed in Sec. 11.2, the conformal transformation of the action (11.45) in BD theories gives rise to a universal coupling Q between a scalar field ϕ and non-relativistic matter in the Einstein frame. For example, the scalaron arising in $f(R)$ gravity has the same coupling $Q = -1/\sqrt{6}$ with any non-relativistic matter species. In the following, we will focus on the universal coupling case by starting from the Jordan-frame action (11.45) with a potential $V(\chi)$ of a scalar field χ .

Performing the conformal transformation $\hat{g}_{\mu\nu} = \chi g_{\mu\nu}$ for the action (11.45), the resulting action in the Einstein frame yields

$$S_E = \int d^4x \sqrt{-\hat{g}} \left[\frac{1}{2} M_{\text{pl}}^2 \hat{R} - \frac{1}{2} (\hat{\nabla}\phi)^2 - \hat{V}(\phi) \right] + \int d^4x L_m(e^{2Q\phi/M_{\text{pl}}} \hat{g}_{\mu\nu}, \Psi_m), \quad (14.1)$$

where ϕ and Q are related to χ and the BD parameter ω_{BD} according to $\chi = e^{-2Q\phi/M_{\text{pl}}}$ and $3 + 2\omega_{\text{BD}} = 1/(2Q^2)$. The potential $V(\chi)$ in the Jordan frame is related to $\hat{V}(\phi)$, as $\hat{V}(\phi) = e^{4Q\phi/M_{\text{pl}}} V(\chi(\phi))$. For the matter sector, we take into account a non-relativistic perfect fluid with density $\hat{\rho}$ and vanishing pressure in the Einstein frame.

Since the trace $\hat{T}_m$ in Eq. (11.68) is given by $\hat{T}_m = -\hat{\rho}$, the scalar-field equation in the Einstein frame reads

$$\hat{\square}\phi - \hat{V}_{,\phi} - \frac{Q}{M_{\text{pl}}} \hat{\rho} = 0. \quad (14.2)$$

On the spherically symmetric background in the Minkowski spacetime, the line element in the Jordan frame is $ds^2 = g_{\mu\nu} dx^\mu dx^\nu = -dt^2 + dr^2 + r^2(d\theta^2 + \sin^2\theta d\varphi^2)$. After the conformal transformation $\hat{g}_{\mu\nu} = e^{-2Q\phi/M_{\text{pl}}} g_{\mu\nu}$, the radial distance $\hat{r}$ in the Einstein frame is transformed as $\hat{r} = e^{-Q\phi/M_{\text{pl}}} r$. From Eq. (11.66), the density ρ in the Jordan frame is related to $\hat{\rho}$, as $\rho = e^{-4Q\phi/M_{\text{pl}}} \hat{\rho}$. If we define the density

$$\rho^* = e^{3Q\phi/M_{\text{pl}}} \rho = e^{-Q\phi/M_{\text{pl}}} \hat{\rho}, \quad (14.3)$$

it satisfies the conserved relation $\rho r^3 = \rho^* \hat{r}^3$. On using this conserved density ρ^* , we can write Eq. (14.2) in the following form:

$$\frac{d^2\phi}{d\hat{r}^2} + \frac{2}{\hat{r}} \frac{d\phi}{d\hat{r}} - \frac{dV_{\text{eff}}(\phi)}{d\phi} = 0, \quad (14.4)$$

where the effective potential is given by

$$V_{\text{eff}}(\phi) = \hat{V}(\phi) + e^{Q\phi/M_{\text{pl}}} \rho^*. \quad (14.5)$$

We consider a runaway positive potential $\hat{V}(\phi)$ in the region $\phi > 0$ that monotonically decreases and has a positive mass squared, i.e., $\hat{V}_{,\phi} < 0$ and $\hat{V}_{,\phi\phi} > 0$ [2]. We also demand the following conditions:

$$\lim_{\phi \rightarrow 0} \left| \frac{\hat{V}_{,\phi}}{\hat{V}} \right| = \infty, \quad \lim_{\phi \rightarrow \infty} \frac{\hat{V}_{,\phi}}{\hat{V}} = 0. \quad (14.6)$$

The former is required to have a large mass in regions of the high density, whereas the latter is required to realize the late-time cosmic acceleration in regions of the low density. As $\phi \rightarrow 0$, the potential $\hat{V}$ approaches either ∞ or a finite positive value V_0 . In the limit that $\phi \rightarrow \infty$, we have either $\hat{V} \rightarrow 0$ or $\hat{V} \rightarrow V_\infty$, where V_∞ is a non-zero positive constant. For $Q > 0$, the effective potential $V_{\text{eff}}(\phi)$ has a minimum at the field value $\phi_m (> 0)$ satisfying the condition $V_{\text{eff},\phi}(\phi_m) = 0$, i.e.

$$\hat{V}_{,\phi}(\phi_m) + Qe^{Q\phi_m/M_{\text{Pl}}} \rho^*/M_{\text{Pl}} = 0. \quad (14.7)$$

If the potential satisfies the conditions $\hat{V}_{,\phi} > 0$ and $\hat{V}_{,\phi\phi} > 0$ in the region $\phi < 0$, there exists a potential minimum at $\phi = \phi_m (< 0)$ for $Q < 0$. As we will see in Sec. 14.1.4.1, this situation arises for $f(R)$ models (11.14)–(11.16). After deriving the field profile and gravitational potentials in a general way, we will apply them to models of the late-time cosmic acceleration based on $f(R)$ gravity and BD theory.

14.1.1. Field profile inside and outside the body

We consider the existence of a spherically symmetric body whose density inside the body ($\hat{r} < \hat{r}_c$) is constant with the value $\rho^* = \rho_A$. We also assume that the density outside the body ($\hat{r} > \hat{r}_c$) has a constant value $\rho^* = \rho_B$ much smaller than ρ_A . The mass of the body and the gravitational potential Φ at radius $\hat{r}_c$ are given, respectively, by $M_c = (4\pi/3)\hat{r}_c^3 \rho_A$ and $\Phi_c = GM_c/\hat{r}_c$. The effective potential (14.5) has two minima at the field values ϕ_A and ϕ_B satisfying

$$\hat{V}_{,\phi}(\phi_A) + Qe^{Q\phi_A/M_{\text{Pl}}} \rho_A/M_{\text{Pl}} = 0, \quad (14.8)$$

$$\hat{V}_{,\phi}(\phi_B) + Qe^{Q\phi_B/M_{\text{Pl}}} \rho_B/M_{\text{Pl}} = 0. \quad (14.9)$$

The former corresponds to the region of high density with a heavy mass squared $m_A^2 \equiv V_{\text{eff},\phi\phi}(\phi_A)$, whereas the latter to a lower density region with a light mass squared $m_B^2 \equiv V_{\text{eff},\phi\phi}(\phi_B)$. For the Sun, we can take the average density $\rho_A \simeq 1 \text{ g/cm}^3$ inside the body and the homogeneous dark matter/baryon density in our galaxy $\rho_B \simeq 10^{-24} \text{ g/cm}^3$ outside the body.

As we see in Eq. (14.4), the inverted effective potential $-V_{\text{eff}}(\phi)$ determines the “dynamics” of the field ϕ . In Fig. 14.1, we illustrate the shape of $-V_{\text{eff}}(\phi)$ inside and outside the spherically symmetric body. To derive the field profile as a function

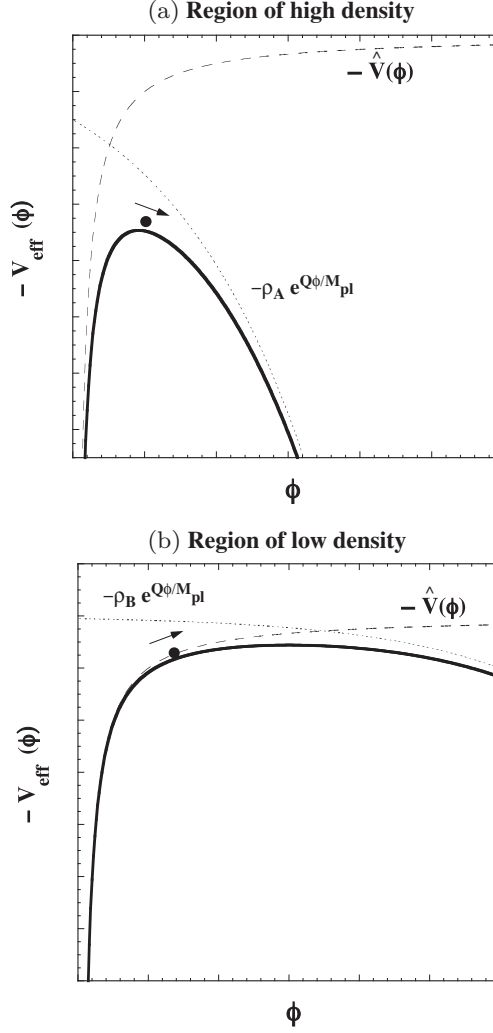


Fig. 14.1. Inverted effective potential $-V_{\text{eff}}(\phi)$ of a chameleon scalar field ϕ inside (top) and outside (bottom) a spherically symmetric body. Inside the body (density ρ_A), the effective potential has an extremum at $\phi = \phi_A$, whereas outside the body (density ρ_B), the extremum exists at $\phi = \phi_B$. Since $\rho_A \gg \rho_B$, it follows that $|\phi_A| \ll |\phi_B|$.

of $\hat{r}$, we impose the boundary conditions at $\hat{r} = 0$ and $\hat{r} \rightarrow \infty$ as

$$\frac{d\phi}{d\hat{r}}(\hat{r} = 0) = 0, \quad (14.10)$$

$$\phi(\hat{r} \rightarrow \infty) = \phi_B. \quad (14.11)$$

The field ϕ is at rest at $\hat{r} = 0$ and starts to roll down the potential when the matter-coupling term $Qe^{Q\phi/M_{\text{pl}}} \rho_A/M_{\text{pl}}$ in Eq. (14.4) becomes important at a radius $\hat{r}_1$. If

the field value at $\hat{r} = 0$ is close to ϕ_A , the field stays around ϕ_A in the region $0 < \hat{r} < \hat{r}_1$. For large density ρ_A , the field value $|\phi_A|$ is close to 0, so we assume the condition $Q\phi_A/M_{\text{pl}} \ll 1$ in the following discussion. If $\hat{r}_1$ is close to the radius $\hat{r}_c$ of the body, the body has a thin-shell in the region $\hat{r}_1 < \hat{r} < \hat{r}_c$ in which the variation of the field occurs.

In the region $0 < \hat{r} < \hat{r}_1$, the derivative $dV_{\text{eff}}/d\phi$ in Eq. (14.4) can be approximated as $dV_{\text{eff}}/d\phi \simeq m_A^2(\phi - \phi_A)$ around $\phi = \phi_A$. Hence the solution to Eq. (14.4) is given by

$$\phi(\hat{r}) = \phi_A + A \frac{e^{-m_A \hat{r}}}{\hat{r}} + B \frac{e^{m_A \hat{r}}}{\hat{r}}, \quad (14.12)$$

where A and B are integration constants. To avoid the divergence of ϕ at $\hat{r} = 0$, we demand the condition $B = -A$. Then, the solution (14.12) yields

$$\phi(\hat{r}) = \phi_A + \frac{A(e^{-m_A \hat{r}} - e^{m_A \hat{r}})}{\hat{r}} \quad (0 < \hat{r} < \hat{r}_1), \quad (14.13)$$

which satisfies the boundary condition (14.10).

The field stays around the potential maximum for $0 < \hat{r} < \hat{r}_1$, but in the regime $\hat{r}_1 < \hat{r} < \hat{r}_c$ it exhibits the variation from $\phi = \phi_A$. Since $|V_{,\phi}| \ll |Qe^{Q\phi/M_{\text{pl}}} \rho_A/M_{\text{pl}}|$ in this regime, we have that $dV_{\text{eff}}/d\phi \simeq Q\rho_A/M_{\text{pl}}$, where we used the condition $Q\phi/M_{\text{pl}} \ll 1$. Then, we obtain the following solution

$$\phi(\hat{r}) = \frac{Q\rho_A}{6M_{\text{pl}}} \hat{r}^2 - \frac{C}{\hat{r}} + D \quad (\hat{r}_1 < \hat{r} < \hat{r}_c), \quad (14.14)$$

where C and D are integration constants.

Outside the body ($\hat{r} > \hat{r}_c$), the shape of the effective potential changes relative to that inside the body due to the drop down of the matter density from ρ_A to ρ_B . The field acquires a sufficient kinetic energy in the region $\hat{r}_1 < \hat{r} < \hat{r}_c$, so it climbs up the potential hill toward the value ϕ_B . Under the condition $\rho_A \gg \rho_B$, we have that $|\phi_B| \gg |\phi_A|$. Expansion of the effective potential around $\phi = \phi_B$ gives $dV_{\text{eff}}/d\phi \simeq m_B^2(\phi - \phi_B)$. Then, we obtain the solution $\phi(\hat{r}) = \phi_B + Ee^{-m_B(\hat{r}-\hat{r}_c)}/\hat{r} + Fe^{m_B(\hat{r}-\hat{r}_c)}/\hat{r}$, where E and F are integration constants. Under the boundary condition (14.11), we require that $F = 0$. Then, the solution yields

$$\phi(\hat{r}) = \phi_B + E \frac{e^{-m_B(\hat{r}-\hat{r}_c)}}{\hat{r}} \quad (\hat{r} > \hat{r}_c). \quad (14.15)$$

The three solutions (14.13), (14.14) and (14.15) should be matched at $\hat{r} = \hat{r}_1$ and $\hat{r} = \hat{r}_c$ by imposing continuity conditions for ϕ and $d\phi/d\hat{r}$. The coefficients C , A , E and D are determined as [4]

$$C = \frac{s_3}{m_A(e^{-m_A \hat{r}_1} + e^{m_A \hat{r}_1})s_2 - m_B s_1}, \quad (14.16)$$

$$A = -\frac{1}{s_1} \left(C + \frac{Q\rho_A \hat{r}_1^3}{3M_{\text{pl}}} \right), \quad (14.17)$$

$$E = -\frac{1}{s_2} \left(C + \frac{Q\rho_A \hat{r}_c^3}{3M_{\text{pl}}} \right), \quad (14.18)$$

$$D = \phi_B - \frac{Q\rho_A}{6M_{\text{pl}}} \hat{r}_c^2 + \frac{1}{\hat{r}_c} (C + E), \quad (14.19)$$

where

$$s_1 = m_A \hat{r}_1 (e^{-m_A \hat{r}_1} + e^{m_A \hat{r}_1}) + e^{-m_A \hat{r}_1} - e^{m_A \hat{r}_1}, \quad (14.20)$$

$$s_2 = 1 + m_B \hat{r}_c, \quad (14.21)$$

$$s_3 = s_1 s_2 \left[\phi_B - \phi_A + (\hat{r}_1^2 - \hat{r}_c^2) \frac{Q\rho_A}{6M_{\text{pl}}} \right] + [s_2 \hat{r}_1^2 (e^{-m_A \hat{r}_1} - e^{m_A \hat{r}_1}) - s_1 \hat{r}_c^2] \frac{Q\rho_A}{3M_{\text{pl}}}. \quad (14.22)$$

If the mass m_B is small such that the conditions $m_B \hat{r}_c \ll 1$ and $m_B \ll m_A$ are satisfied, we can neglect contributions of the m_B -dependent terms in Eqs. (14.16)–(14.19). Then, the field profile is given by

$$\phi(\hat{r}) = \phi_A - \frac{1}{m_A(e^{-m_A \hat{r}_1} + e^{m_A \hat{r}_1})} \left[\phi_B - \phi_A + \frac{Q\rho_A}{2M_{\text{pl}}} (\hat{r}_1^2 - \hat{r}_c^2) \right] \frac{e^{-m_A \hat{r}} - e^{m_A \hat{r}}}{\hat{r}},$$

(for $0 < \hat{r} < \hat{r}_1$), (14.23)

$$\phi(\hat{r}) = \phi_B + \frac{Q\rho_A}{6M_{\text{pl}}} (\hat{r}^2 - 3\hat{r}_c^2) + \frac{Q\rho_A \hat{r}_1^3}{3M_{\text{pl}} \hat{r}} - \left[1 + \frac{e^{-m_A \hat{r}_1} - e^{m_A \hat{r}_1}}{m_A \hat{r}_1 (e^{-m_A \hat{r}_1} + e^{m_A \hat{r}_1})} \right] \left[\phi_B - \phi_A + \frac{Q\rho_A}{2M_{\text{pl}}} (\hat{r}_1^2 - \hat{r}_c^2) \right] \frac{\hat{r}_1}{\hat{r}},$$

(for $\hat{r}_1 < \hat{r} < \hat{r}_c$), (14.24)

$$\phi(\hat{r}) = \phi_B - \left[\hat{r}_1 (\phi_B - \phi_A) + \frac{Q\rho_A}{6M_{\text{pl}}} \hat{r}_c^3 \left(2 + \frac{\hat{r}_1}{\hat{r}_c} \right) \left(1 - \frac{\hat{r}_1}{\hat{r}_c} \right)^2 + \frac{e^{-m_A \hat{r}_1} - e^{m_A \hat{r}_1}}{m_A (e^{-m_A \hat{r}_1} + e^{m_A \hat{r}_1})} \left\{ \phi_B - \phi_A + \frac{Q\rho_A}{2M_{\text{pl}}} (\hat{r}_1^2 - \hat{r}_c^2) \right\} \right] \frac{e^{-m_B (\hat{r} - \hat{r}_c)}}{\hat{r}},$$

(for $\hat{r} > \hat{r}_c$). (14.25)

The radius r_1 is determined by the condition

$$m_A^2 [\phi(\hat{r}_1) - \phi_A] = \frac{Q\rho_A}{M_{\text{pl}}}, \quad (14.26)$$

which translates to

$$\phi_B - \phi_A + \frac{Q\rho_A}{2M_{\text{pl}}}(\hat{r}_1^2 - \hat{r}_c^2) = \frac{6QM_{\text{pl}}\Phi_c}{(m_A\hat{r}_c)^2} \frac{m_A\hat{r}_1(e^{m_A\hat{r}_1} + e^{-m_A\hat{r}_1})}{e^{m_A\hat{r}_1} - e^{-m_A\hat{r}_1}}, \quad (14.27)$$

where $\Phi_c = GM_c/\hat{r}_c = \rho_A\hat{r}_c^2/(6M_{\text{pl}}^2)$ is the gravitational potential at the surface of body. Using this relation, the field profile (14.25) outside the body reads

$$\phi(\hat{r}) = \phi_B - 2Q_{\text{eff}}M_{\text{pl}}\Phi_c \frac{\hat{r}_c e^{-m_B(\hat{r}-\hat{r}_c)}}{\hat{r}}, \quad (14.28)$$

where

$$Q_{\text{eff}} \equiv Q \left[1 - \frac{\hat{r}_1^3}{\hat{r}_c^3} + 3 \frac{\hat{r}_1}{\hat{r}_c} \frac{1}{(m_A\hat{r}_c)^2} \left\{ \frac{m_A\hat{r}_1(e^{m_A\hat{r}_1} + e^{-m_A\hat{r}_1})}{e^{m_A\hat{r}_1} - e^{-m_A\hat{r}_1}} - 1 \right\} \right]. \quad (14.29)$$

As we will see below, the quantity Q_{eff} characterizes the effective gravitational coupling with matter mediated by the scalar field ϕ . In the limit that $\hat{r}_1 \rightarrow 0$, the effective coupling Q_{eff} is equivalent to the bare coupling Q .

On the other hand, if $\hat{r}_1$ is close to $\hat{r}_c$ such that the condition $\Delta\hat{r}_c \equiv \hat{r}_c - \hat{r}_1 \ll \hat{r}_c$ is satisfied, the body has a thin shell in which the variation of the field occurs for the distance $\hat{r}_1 < \hat{r} < \hat{r}_c$. Provided that the field is sufficiently massive inside the body such that the condition $m_A\hat{r}_c \gg 1$ is satisfied, the expansion of Eq. (14.29) gives

$$Q_{\text{eff}} = 3Q \left(\frac{\Delta\hat{r}_c}{\hat{r}_c} + \frac{1}{m_A\hat{r}_c} \right). \quad (14.30)$$

In this case, the effective coupling $|Q_{\text{eff}}|$ is much smaller than $|Q|$. From Eq. (14.27), we also have the following relation:

$$\epsilon_{\text{th}} \equiv \frac{\phi_B - \phi_A}{6QM_{\text{pl}}\Phi_c} \simeq \frac{\Delta\hat{r}_c}{\hat{r}_c} + \frac{1}{m_A\hat{r}_c}, \quad (14.31)$$

where ϵ_{th} is called the thin-shell parameter characterizing the strength of effective coupling Q_{eff} [1, 2]. From Eqs. (14.23) and (14.24), the field values at $\hat{r} = 0$ and $\hat{r} = \hat{r}_1$ are given, respectively, by

$$\phi(0) \simeq \phi_A + \frac{12Q\Phi_c}{m_A\hat{r}_c e^{m_A\hat{r}_c}}, \quad (14.32)$$

$$\phi(\hat{r}_1) \simeq \phi_A + \frac{6Q\Phi_c}{(m_A\hat{r}_c)^2}. \quad (14.33)$$

Under the condition $m_A\hat{r}_c \gg 1$, the field $\phi(r)$ is very close to ϕ_A for the distance $\hat{r} \leq \hat{r}_1$. Hence the variation of $\phi(r)$ occurs only in the thin-shell region, which leads to the suppression of fifth forces outside the body. Taking the massless limit $m_B \rightarrow 0$

in Eq. (14.28) and using the approximation $|\phi_B| \gg |\phi_A|$ in Eq. (14.31), the solution (14.28) outside the body can be expressed as

$$\phi(\hat{r}) \simeq 6QM_{\text{pl}}\Phi_c\epsilon_{\text{th}} \left(1 - \frac{\hat{r}_c}{\hat{r}}\right), \quad (14.34)$$

which approaches $\phi_B \simeq 6QM_{\text{pl}}\Phi_c\epsilon_{\text{th}}$ as $\hat{r} \rightarrow \infty$.

14.1.2. *Post-Newtonian parameter*

Existence of a chameleon scalar field gives rise to the fifth force due to the modifications of two gravitational potentials Ψ and Φ . This also induces the deviation of the gravitational slip parameter $\gamma = -\Phi/\Psi$ from 1. We derive the bound on the thin-shell parameter from experimental tests of the post-Newtonian parameter γ around the body with mass M_c . We take the spherically symmetric metric in the Einstein frame in the form [5]

$$ds^2 = \hat{g}_{\mu\nu} d\hat{x}^\mu d\hat{x}^\nu = -[1 + 2\hat{\Psi}(\hat{r})]dt^2 + [1 + 2\hat{\Phi}(\hat{r})]d\hat{r}^2 + \hat{r}^2 d\Omega^2, \quad (14.35)$$

where $\hat{\Psi}(\hat{r})$ and $\hat{\Phi}(\hat{r})$ are functions of $\hat{r}$ and $d\Omega^2 = d\theta^2 + \sin^2\theta d\varphi^2$. Ignoring the energy density of the field $\phi(\hat{r})$, we can approximate the region outside the body as a vacuum. Then, the corresponding spacetime in the Einstein frame is given by the Schwarzschild vacuum solution with mass M_c . In the weak-field limit ($|\hat{\Psi}| \ll 1$ and $|\hat{\Phi}| \ll 1$), the gravitational potentials outside the body are given by

$$\hat{\Psi}(\hat{r}) \simeq -\frac{GM_c}{\hat{r}}, \quad \hat{\Phi}(\hat{r}) \simeq \frac{GM_c}{\hat{r}}. \quad (14.36)$$

We transform the metric (14.35) back to that in the Jordan frame under the inverse conformal transformation, $g_{\mu\nu} = e^{2Q\phi/M_{\text{pl}}} \hat{g}_{\mu\nu}$. The metric in the Jordan frame, $ds^2 = e^{2Q\phi/M_{\text{pl}}} d\hat{s}^2 = g_{\mu\nu} dx^\mu dx^\nu$, is given by

$$ds^2 = -[1 + 2\Psi(r)]dt^2 + [1 + 2\Phi(r)]dr^2 + r^2 d\Omega^2, \quad (14.37)$$

where $r = e^{Q\phi/M_{\text{pl}}} \hat{r}$. Under the condition $|Q\phi/M_{\text{pl}}| \ll 1$, it follows that

$$\Psi(r) \simeq \hat{\Psi}(\hat{r}) + \frac{Q\phi(\hat{r})}{M_{\text{pl}}} = -\frac{GM_c}{\hat{r}} + \frac{Q\phi(\hat{r})}{M_{\text{pl}}}, \quad (14.38)$$

$$\Phi(r) \simeq \hat{\Phi}(\hat{r}) - \frac{Q}{M_{\text{pl}}} \hat{r} \frac{d\phi(\hat{r})}{d\hat{r}} = \frac{GM_c}{\hat{r}} - \frac{Q}{M_{\text{pl}}} \hat{r} \frac{d\phi(\hat{r})}{d\hat{r}}. \quad (14.39)$$

Substituting the thin-shell solution (14.34) into Eqs. (14.38)–(14.39) and using the approximation $\hat{r} \simeq r$, we obtain

$$\Psi(r) \simeq -\frac{GM_c}{r} \left[1 + 6Q^2\epsilon_{\text{th}} \left(1 - \frac{r}{r_c}\right)\right], \quad (14.40)$$

$$\Phi(r) \simeq \frac{GM_c}{r} (1 - 6Q^2\epsilon_{\text{th}}). \quad (14.41)$$

In the limit of weak gravity, a free-falling particle with a unit mass obeys the equation of motion (3.71), where $h_{00} = -2\Psi(r)$. Then, the gravitational force exerted on the particle is given by $F^i = \partial^i h_{00}/2 = -\partial^i \Psi$. On using the solution (14.40), the equation in the radial direction yields

$$\ddot{r} = -\frac{GM_c}{r^2} (1 + 6Q^2\epsilon_{\text{th}}). \quad (14.42)$$

In addition to the Newtonian gravitational force $F_0 = -GM_c/r^2$, there exists the extra (fifth) force $6Q^2\epsilon_{\text{th}}F_0$. Provided that the chameleon mechanism is at work such that the condition $\epsilon_{\text{th}} \ll 1$ is satisfied, the fifth force is suppressed to recover the Newton gravity.

The difference between two gravitational potentials is quantified by the post-Newtonian parameter $\gamma = -\Phi/\Psi$. From Eqs. (14.40) and (14.41), we have

$$\gamma \simeq \frac{1 - 6Q^2\epsilon_{\text{th}}}{1 + 6Q^2\epsilon_{\text{th}}(1 - r/r_c)}. \quad (14.43)$$

In the limit that $\epsilon_{\text{th}} \rightarrow 0$, Eq. (14.43) reduces to the value of GR ($\gamma = 1$). From the time-delay effect of the Cassini tracking of the Sun, there is the following experimental bound [6]

$$|\gamma - 1| < 2.3 \times 10^{-5}. \quad (14.44)$$

Taking the distance $r = r_c$ in Eq. (14.43), the constraint (14.44) translates to

$$\epsilon_{\odot} < \frac{3.8 \times 10^{-6}}{Q^2}, \quad (14.45)$$

where $\epsilon_{\odot}$ is the thin-shell parameter of the Sun. In $f(R)$ gravity ($Q = -1/\sqrt{6}$), the bound (14.45) corresponds to $\epsilon_{\odot} < 2.3 \times 10^{-5}$.

14.1.1.3. Violation of equivalence principle

We discuss local gravity constraints coming from the possible violation of equivalence principle. If the Earth has a thin shell, the effective coupling Q_{eff} outside the body is given by $Q_{\text{eff}} = 3Q\epsilon_{\oplus}$, where $\epsilon_{\oplus}$ is the thin-shell parameter of the Earth. Under the situation where the Sun (mass $M_{\odot}$) also has a thin shell, the acceleration exerted on the Earth from the Sun in the radial direction is given by

$$a_{\oplus} = -\frac{d\Psi(r)}{dr} \simeq -\frac{GM_{\odot}}{r^2} - \frac{3Q\epsilon_{\oplus}}{M_{\text{pl}}} \frac{d\phi}{dr}, \quad (14.46)$$

where, in Eq. (14.38), we replaced the term Q with $3Q\epsilon_{\oplus}$ and used the approximation $\hat{r} \simeq r$. On using the solution (14.34), the field profile outside the Sun reads $\phi(r) \simeq 6QM_{\text{pl}}\Phi_{\odot}\epsilon_{\odot}(1 - r_c/r)$, where $\Phi_{\odot} \simeq 2.1 \times 10^{-6}$ is the gravitational of the Sun. Substituting this field profile into Eq. (14.46), it follows that

$$a_{\oplus} = -\frac{GM_{\odot}}{r^2} (1 + 18Q^2\epsilon_{\oplus}\epsilon_{\odot}). \quad (14.47)$$

Similarly, if the Moon has a thin shell with a thin-shell parameter ϵ_M , the acceleration induced from the Sun in the radial direction is given by

$$a_M = -\frac{GM_\odot}{r^2} (1 + 18Q^2\epsilon_M\epsilon_\odot). \quad (14.48)$$

Taking $\rho_B \simeq 10^{-24} \text{ g/cm}^3$ as a mean density of our galaxy for Earth, Sun, and Moon, their thin-shell parameters are given, respectively, by $\epsilon_\oplus \simeq \phi_B/(6QM_{\text{pl}}\Phi_\oplus)$, $\epsilon_\odot \simeq \phi_B/(6QM_{\text{pl}}\Phi_\odot)$, and $\epsilon_M \simeq \phi_B/(6QM_{\text{pl}}\Phi_M)$, where $\Phi_\oplus \simeq 7.0 \times 10^{-10}$ and $\Phi_M \simeq 3.1 \times 10^{-11}$. Then, we have the relations $\epsilon_\odot \simeq (\Phi_\oplus/\Phi_\odot)\epsilon_\oplus$ and $\epsilon_M \simeq (\Phi_\oplus/\Phi_M)\epsilon_\oplus$. Then, Eqs. (14.47) and (14.48) reduce, respectively, to [2]

$$a_\oplus \simeq -\frac{GM_\odot}{r^2} \left[1 + 18Q^2\epsilon_\oplus^2 \frac{\Phi_\oplus}{\Phi_\odot} \right], \quad (14.49)$$

$$a_M \simeq -\frac{GM_\odot}{r^2} \left[1 + 18Q^2\epsilon_\oplus^2 \frac{\Phi_\oplus^2}{\Phi_\odot\Phi_M} \right]. \quad (14.50)$$

From local gravity tests, the difference between $a_\oplus$ and a_M is constrained to be [6, 7]

$$\frac{|a_\oplus - a_M|}{|a_\oplus + a_M|/2} < 10^{-13}. \quad (14.51)$$

From Eqs. (14.49) and (14.50), the bound (14.51) translates to

$$\epsilon_\oplus < \frac{8.8 \times 10^{-7}}{|Q|}. \quad (14.52)$$

In $f(R)$ gravity, the bound (14.52) corresponds to $\epsilon_\oplus < 2.2 \times 10^{-6}$.

Since $\epsilon_\oplus \simeq \phi_B/(6QM_{\text{pl}}\Phi_\oplus)$ under the condition $|\phi_B| \gg |\phi_A|$, the bound (14.52) also translates to

$$|\phi_B| < 3.7 \times 10^{-15} M_{\text{pl}}, \quad (14.53)$$

which can be used to put constraints on concrete models of the late-time cosmic acceleration.

14.1.4. Local gravity constraints on $f(R)$ gravity and Brans–Dicke theory

14.1.4.1. $f(R)$ gravity

We first discuss local gravity constraints on $f(R)$ models given by Eqs. (11.14) and (11.15) [5, 8–10]. In the region where R is much larger than $R_0 \approx H_0^2$, these models have the asymptotic form (11.17). We recall that the scalar field ϕ and the potential $\hat{V}(\phi)$ in the Einstein frame are given, respectively, by Eqs. (11.80) and (11.81).

On using Eq. (11.17), the effective potential $V_{\text{eff}}(\phi)$ outside the spherically symmetric body has a minimum at

$$\phi_B \simeq -\sqrt{6}n\lambda \left(\frac{M_{\text{pl}}^2 R_0}{\rho_B} \right)^{2n+1} M_{\text{pl}}, \quad (14.54)$$

which is negative. The experimental bound (14.53) translates to

$$n\lambda \left(\frac{M_{\text{pl}}^2 R_0}{\rho_B} \right)^{2n+1} < 1.5 \times 10^{-15}. \quad (14.55)$$

The model (11.17) has a de Sitter fixed point at $R = R_1$. We focus on the case in which the Lagrangian density is given by Eq. (11.17) for $R \geq R_1$. The local gravity constraints on the original models (11.14) and (11.15) are similar to those discussed below.

For the model (11.17), there is the relation $\lambda = x_1^{2n+1}/[2(x_1^{2n} - n - 1)]$, where $x_1 = R_1/R_0$ and R_1 is the Ricci scalar at the de Sitter solution. Substituting this relation into Eq. (14.55), we obtain

$$\frac{n}{2(x_1^{2n} - n - 1)} \left(\frac{M_{\text{pl}}^2 R_1}{\rho_B} \right)^{2n+1} < 1.5 \times 10^{-15}. \quad (14.56)$$

The stability of the de Sitter fixed point is ensured under the condition (11.32), which translates to the condition $x_1^{2n} > 2n^2 + 3n + 1$. Then, the term $n/[2(x_1^{2n} - n - 1)]$ in Eq. (14.56) is smaller than 0.25 for $n > 0$. We employ the approximation that $M_{\text{pl}}^2 R_1$ and ρ_B are of the orders of the present cosmological density 10^{-29} g/cm^3 and the baryonic/dark matter density 10^{-24} g/cm^3 in our galaxy, respectively. From the bound (14.56), the power n is constrained to be [10]

$$n > 0.9. \quad (14.57)$$

We note that the constraint (14.45) from the Cassini tracking gives a weaker bound on n . The above results show that the $f(R)$ dark energy models (11.14) and (11.15) can be consistent with local gravity constraints for $n \geq 1$, while showing a deviation from the Λ CDM model on cosmological scales.

14.1.4.2. Brans–Dicke theories

We also study local gravity constraints on BD theory (11.63) with the potential (12.125) in the Jordan frame. The potential in the Einstein frame is given by $\hat{V}(\phi) = e^{4Q\phi/M_{\text{pl}}} V(\phi)$, i.e.,

$$\hat{V}(\phi) = e^{4Q\phi/M_{\text{pl}}} V_0 \left[1 - C(1 - e^{-2Q\phi/M_{\text{pl}}})^p \right], \quad (14.58)$$

where $0 < p < 1$. Since $\hat{V}_{,\phi} \simeq -V_0 C p (2Q/M_{\text{pl}})^p \phi^{p-1}$ under the condition $|Q\phi| \ll 1$, the field value ϕ_B outside the body yields

$$\phi_B \simeq \frac{M_{\text{pl}}}{2Q} \left(\frac{2p C V_0}{\rho_B} \right)^{1/(1-p)}. \quad (14.59)$$

The experimental bound (14.53) translates to

$$\left(\frac{2p C V_0}{\rho_B} \right)^{1/(1-p)} < 7.4 \times 10^{-15} |Q|. \quad (14.60)$$

We consider the case in which the cosmological solution finally approaches a de Sitter fixed point explained in Sec. 11.2.2. At this de Sitter point, we have $3M_{\text{pl}}^2 F_{\text{dS}} H_{\text{dS}}^2 = V_0 [1 - C(1 - F_{\text{dS}})^p]$, where the constant C satisfies Eq. (11.97). Then, we obtain the following relation

$$V_0 = \frac{3M_{\text{pl}}^2 H_{\text{dS}}^2}{p} [2 + (p - 2)F_{\text{dS}}]. \quad (14.61)$$

The bound (14.60) translates to

$$\left(\frac{M_{\text{pl}}^2 R_{\text{dS}}}{\rho_B} \right)^{1/(1-p)} (1 - F_{\text{dS}}) < 7.4 \times 10^{-15} |Q|, \quad (14.62)$$

where $R_{\text{dS}} = 12H_{\text{dS}}^2$ is the Ricci scalar at the de Sitter point. From Eq. (11.99), the quantity $(1 - F_{\text{dS}})$ is smaller than $1/2$, so the constraint (14.62) gives $(M_{\text{pl}}^2 R_{\text{dS}}/\rho_B)^{1/(1-p)} < 1.5 \times 10^{-14} |Q|$. On using the values $M_{\text{pl}}^2 R_{\text{dS}} \simeq 10^{-29} \text{ g/cm}^3$ and $\rho_B \simeq 10^{-24} \text{ g/cm}^3$, we obtain the following bound [11]

$$p > 1 - \frac{5}{13.8 - \log_{10} |Q|}, \quad (14.63)$$

whose region is plotted as “EP” in Fig. 14.2. If $|Q| = 10^{-1}$ and $|Q| = 1$, then Eq. (14.63) reduce to $p > 0.662$ and $p > 0.638$, respectively. The $f(R)$ models discussed in Sec. 14.1.4.1 correspond to $Q = -1/\sqrt{6}$ and $p = 2n/(2n + 1)$, so the bound (14.63) translates to $p > 0.648$, i.e., $n > 0.9$. The Cassini tracking constraint (14.45) gives a weaker bound on p than that given by Eq. (14.63), see Fig. 14.2.

In Fig. 14.2, we plot two bounds arising from the growth of matter density perturbations discussed in Sec. 12.4.2. Provided that p satisfies the bound (14.63) and $|Q|$ is smaller than the order of unity, there exists the viable parameter space consistent with both local gravity and cosmological constraints. In the above discussions, we have employed the two local gravity bounds (14.44) and (14.51), but it is possible to place constraints on the model parameters further by using the Eöt–Wash experiment [12], the Lunar Laser Ranging experiment [6], and the CMB constraint on the time-variation of particle masses [13]. In Ref. [14], it was shown that the potential (12.125) is also consistent with those bounds for p closer to 1.

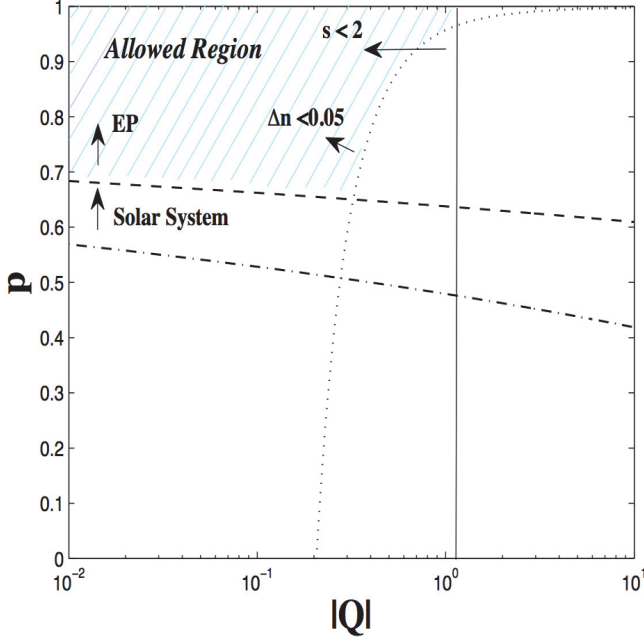


Fig. 14.2. Allowed parameter space in the (p, Q) plane in BD theory (11.63) with the potential (12.125). The bounds shown as “EP” and “Solar System” are those from the local gravity constraints (14.52) and (14.45), respectively. We also plot the cosmological bounds $s < 2$ and $\Delta n < 0.05$, where $s = \delta_m/(H\delta_m)$ and Δn is the difference between the spectral indices of the matter power spectrum and the CMB spectrum. Reproduced from Ref. [11].

Readers may refer to the references [15–23] for other experimental and cosmological aspects of chameleons.

14.2. Vainshtein mechanism in scalar–tensor theories with non-linear derivative couplings

Besides the chameleon mechanism, there is another way of screening fifth forces called the Vainshtein mechanism [3] based on non-linear field derivative interactions.

Originally, the Vainshtein mechanism was proposed in the context of Pauli–Fierz massive gravity with a Lorentz-invariant massive spin-2 field $h_{\mu\nu}$ [24]. The quadratic Pauli–Fierz theory, expanded up to second order in $h_{\mu\nu}$, possesses a so-called van Dam–Veltman–Zakharov (vDVZ) discontinuity [25, 26] with which the linearized GR is not recovered in the limit that the graviton mass is sent to zero. Vainshtein showed that, in a non-linear version of Pauli–Fierz theory, there is a regular expansion valid within a radius r_V (called the Vainshtein radius) [3]. Thus, the non-linearities arising from the expansion in terms of $h_{\mu\nu}$ higher than second order allow the possibility for recovering the behavior close to GR [27–29]. Unfortunately the non-linearities that cure the vDVZ discontinuity problem give

rise to a so-called Boulware–Deser (BD) ghost [30], but de Rham, Gabadadze, and Tolley (dRGT) constructed a non-linear massive gravity theory free from the BD ghost [31]. Later, it was shown that all isotropic and homogeneous cosmological solutions in the dRGT massive gravity are unstable [32, 33], so the original dRGT model itself cannot be used as a viable dark energy scenario.

As we mentioned in Sec. 11.3, the DGP braneworld [34] offers a possibility for realizing the late-time cosmic acceleration by a gravitational leakage to the extra dimension. The DGP model contains a ghost mode in addition to the incompatibility with the observational data of SN Ia, BAO, and CMB, but it has a nice feature to recover the behavior close to GR in a local region due to the appearance of a non-linear field derivative interaction $X\Box\phi$ [35, 36]. This non-linear term arises as a result of the mixture of a transverse graviton with a brane-bending (longitudinal) mode ϕ . This longitudinal mode has a non-minimal coupling to the four-dimensional Ricci scalar R on the brane in the form $e^{-2Q\phi/M_{\text{Pl}}}R$, but the non-linear derivative interaction suppresses the propagation of fifth forces for the distance smaller than the Vainshtein radius r_V .

The covariant Galileon [37] contains derivative interactions more general than the term $X\Box\phi$. In the presence of the non-minimal coupling $e^{-2Q\phi/M_{\text{Pl}}}R$ or in the presence of the scalar-matter coupling (which corresponds to the description in the Einstein frame) with the Einstein–Hilbert term R , both the cubic and the quartic Galileon terms can lead to the recovery of GR within the Vainshtein radius [38–47]. In this section, we will study how the Vainshtein mechanism is at work due to the existence of such derivative interactions in the framework of scalar–tensor theories with one scalar degree of freedom.

For generality, we consider Horndeski theories given by the action (12.13) with (12.1) on a spherically symmetric and static background. We consider the non-minimal coupling $M_{\text{Pl}}^2 e^{-2Q\phi/M_{\text{Pl}}}R/2$ in the Jordan frame by assuming that the matter sector (density ρ and pressure P) is described by a perfect fluid minimally coupled to gravity. Physically, this is equivalent to introducing a coupling Q between matter and a scalar field in the Einstein frame.

14.2.1. *Equations of motion on the spherically symmetric background*

We begin with the line element on the spherically symmetric and static background given by

$$ds^2 = -e^{2\Psi(r)}dt^2 + e^{2\Phi(r)}dr^2 + r^2d\Omega^2, \quad (14.64)$$

where $\Psi(r)$ and $\Phi(r)$ are functions of the distance r from the center of symmetry. To derive the equations of motion, we may write the metric in a more general form $ds^2 = -e^{2\Psi(r)}dt^2 + e^{2\Phi(r)}dr^2 + r^2e^{2\zeta(r)}d\Omega^2$ and express the action (12.13) in terms of Ψ, Φ, ζ, ϕ . Varying the corresponding action with respect to Ψ, Φ, ζ and setting

$\zeta = 0$ in the end, we obtain

$$\left(A_1 + \frac{A_2}{r} + \frac{A_3}{r^2}\right) \Phi' + A_4 + \frac{A_5}{r} + \frac{A_6}{r^2} = e^{2\Phi} \rho, \quad (14.65)$$

$$\left(A_1 + \frac{A_2}{r} + \frac{A_3}{r^2}\right) \Psi' + A_7 + \frac{2A_1}{r} + \frac{A_2 + 2A_8}{2r^2} = e^{2\Phi} P, \quad (14.66)$$

$$\begin{aligned} & \left(-e^{-2\Phi} A_8 + \frac{A_9}{r}\right) (\Psi'' + \Psi'^2) - \left[\left(\frac{A_2}{2} + \frac{A_3 + e^{2\Phi} A_9}{r}\right) \Psi' + A_1 + \frac{A_2}{2r}\right] \Phi' \\ & - \left(\frac{A_5}{2} + \frac{A_6 - A_{10}}{r}\right) \Psi' - A_4 - \frac{A_5}{2r} = e^{2\Phi} P, \end{aligned} \quad (14.67)$$

where a prime represents the derivative with respect to r . The coefficients A_i ($i = 1, 2, \dots, 10$) are given, respectively, by

$$\begin{aligned} A_1 &= -2\phi' X G_{3,X} + 2\phi' (G_{4,\phi} + 2X G_{4,\phi X}), \\ A_2 &= 4G_4 - 16X (G_{4,X} + X G_{4,XX}) + 4X (3G_{5,\phi} + 2X G_{5,\phi X}), \\ A_3 &= 2\phi' (5e^{-2\Phi} - 1) X G_{5,X} + 4\phi' e^{-2\Phi} X^2 G_{5,XX}, \\ A_4 &= G_2 e^{2\Phi} - 2\phi'' (G_{4,\phi} + 2X G_{4,\phi X}) - 2e^{2\Phi} X G_{3,\phi} + 2X G_{3,X} \phi'' + 4e^{2\Phi} X G_{4,\phi\phi}, \\ A_5 &= -4\phi' (G_{4,\phi} - 2X G_{4,\phi X}) - 4\phi' \phi'' e^{-2\Phi} (G_{4,X} + 2X G_{4,XX} \\ & \quad - G_{5,\phi} - X G_{5,\phi X}) - 4\phi' X G_{5,\phi\phi}, \\ A_6 &= -2(1 - e^{2\Phi}) G_4 + 4X G_{4,X} - 2X \{(1 + e^{2\Phi}) G_{5,\phi} - 2X G_{5,\phi X}\} \\ & \quad + 2\phi'' X \{(1 - 3e^{-2\Phi}) G_{5,X} - 2e^{-2\Phi} X G_{5,XX}\}, \\ A_7 &= -e^{2\Phi} (G_2 - 2X G_{2,X} + 2X G_{3,\phi}), \\ A_8 &= -2e^{2\Phi} (G_4 - 2X G_{4,X} + X G_{5,\phi}), \\ A_9 &= 2\phi' e^{-2\Phi} X G_{5,X}, \\ A_{10} &= 2e^{2\Phi} (G_4 - X G_{5,\phi}) + 2\phi'' X G_{5,X}, \end{aligned} \quad (14.68)$$

where $X = -e^{-2\Phi} \phi'^2/2$. The perfect fluid obeys the continuity equation

$$P' + \Psi'(\rho + P) = 0. \quad (14.69)$$

Variation of the action (12.13) with respect to ϕ leads to the scalar-field equation of motion. Differentiating Eq. (14.66) with respect to r and substituting it into Eq. (14.69) with Eqs. (14.65) and (14.67), the same scalar-field equation also follows.

In GR without the scalar field ϕ we have $G_2 = G_3 = G_5 = 0$ and $G_4 = M_{\text{pl}}^2/2$, so Eqs. (14.65) and (14.66) reduce, respectively, to

$$\frac{2M_{\text{pl}}^2}{r}\Phi'_{\text{GR}} - \frac{M_{\text{pl}}^2}{r^2}(1 - e^{2\Phi_{\text{GR}}}) = e^{2\Phi_{\text{GR}}}\rho, \quad (14.70)$$

$$\frac{2M_{\text{pl}}^2}{r}\Psi'_{\text{GR}} + \frac{M_{\text{pl}}^2}{r^2}(1 - e^{2\Phi_{\text{GR}}}) = e^{2\Phi_{\text{GR}}}P. \quad (14.71)$$

The Schwarzschild vacuum solutions to Eqs. (14.70) and (14.71) around a point source with mass M_c are given by $e^{2\Psi} = e^{-2\Phi} = 1 - r_g/r$, where $r_g = M_c/(4\pi M_{\text{pl}}^2)$ is the Schwarzschild radius. If a star has a constant density ρ with a negligible pressure P , then integrations of Eqs. (14.70) and (14.71) give rise to Schwarzschild interior solutions (which we will derive later in Sec. 14.3).

To recover the behavior of gravitational potentials close to that of GR on a weak gravitational background, the dominant contributions to Eqs. (14.65) and (14.66) should be of the orders of $G_4\Phi/r^2$. To quantify corrections to leading-order terms in Eqs. (14.65) and (14.66), we define [43, 47]

$$\begin{aligned} \varepsilon_{G2} &= \frac{e^{2\Phi}G_2r^2}{2G_4}, & \varepsilon_{G2\phi} &= \frac{e^{2\Phi}G_{2,\phi}\phi'r^3}{2G_4}, & \varepsilon_{G2X} &= -\frac{e^{2\Phi}XG_{2,X}r^2}{G_4}, \\ \varepsilon_P &= \frac{e^{2\Phi}Pr^2}{2G_4}, & \varepsilon_{G3\phi} &= -\frac{e^{2\Phi}XG_{3,\phi}r^2}{G_4}, & \varepsilon_{G3X} &= -\frac{XG_{3,X}\phi'r}{G_4}, \\ \varepsilon_{G4\phi} &= \frac{r\phi'G_{4,\phi}}{G_4}, & \varepsilon_{G4X} &= \frac{2XG_{4,X}}{G_4}, & \varepsilon_{G5\phi} &= \frac{XG_{5,\phi}}{2G_4}, \\ \varepsilon_{G5X} &= \frac{e^{-2\Phi}XG_{5,X}\phi'}{2G_4r}, \end{aligned} \quad (14.72)$$

whose orders are required to be much smaller than 1 for realizing solutions close to that of GR. As for the terms containing second derivatives of ϕ or X , say, $G_{4,\phi\phi}$, $G_{4,\phi X}$, $G_{4,XX}$, we introduce the following dimensionless parameters

$$\begin{aligned} \lambda_{G4\phi\phi} &= \frac{G_{4,\phi\phi}\phi'r}{G_{4,\phi}}, & \lambda_{G4\phi X} &= \frac{G_{4,\phi X}\phi'r}{G_{4,X}}, & \lambda_{G4XX} &= \frac{XG_{4,XX}}{G_{4,X}}, \\ \lambda_{G5\phi\phi} &= \frac{G_{5,\phi\phi}\phi'r}{G_{5,\phi}}, & \lambda_{G5\phi X} &= \frac{G_{5,\phi X}\phi'r}{G_{5,X}}, & \lambda_{G5XX} &= \frac{XG_{5,XX}}{G_{5,X}}, \end{aligned} \quad (14.73)$$

etc. These parameters are not necessarily much smaller than 1.

In the following, we expand Eqs. (14.65)–(14.67) in terms of the small parameters (14.72) on the weak gravitational background satisfying the conditions $|\Psi| \ll 1$, $|\Phi| \ll 1$. From Eq. (14.65), the matter density ρ is of the order of $(G_4/r^2)\Phi$. From the continuity equation (14.69), we have $P/\rho \sim \Psi$ and hence $\varepsilon_P \sim \Psi\Phi$. We keep only first-order terms of ε_i by neglecting the contribution of gravitational potentials

higher than first order (such as Ψ^2 and Φ^2). The quantities (14.73) are not dealt with as small expansion parameters.

From Eqs. (14.65)–(14.67), we can eliminate the terms Ψ' and Φ' to give

$$\square\Psi \simeq \mu_1\rho + \mu_2\square\phi + \mu_3, \quad (14.74)$$

where $\square = d^2/dr^2 + (2/r)(d/dr)$, and

$$\mu_1 = \frac{1}{8G_4} \left[2 + 6\Phi + \varepsilon_{G2} + \varepsilon_{G2X} - \varepsilon_{G3\phi} - \varepsilon_{G3X} - (\lambda_{G4\phi X} - 2\lambda_{G4XX} - 3)\varepsilon_{G4X} \right. \\ \left. - \varepsilon_{G4\phi} - 8\varepsilon_{G5\phi} + (2\lambda_{G5\phi X} - 4\lambda_{G5XX} - 12)\varepsilon_{G5X} \right], \quad (14.75)$$

$$\mu_2 = -\frac{\varepsilon_{G3X} + \varepsilon_{G4\phi} + \lambda_{G4\phi X}\varepsilon_{G4X} - 4(1 + \lambda_{G5XX})\varepsilon_{G5X}}{2\phi'r}, \quad (14.76)$$

$$\mu_3 = \frac{2\varepsilon_{G2} + \varepsilon_{G2X} - \lambda_{G4\phi\phi}\varepsilon_{G4\phi} + 2\lambda_{G4XX}\varepsilon_{G4X} + 4(\lambda_{G5\phi X} - 2\lambda_{G5XX} - 2)\varepsilon_{G5X}}{2r^2}. \quad (14.77)$$

On using Eqs. (14.65)–(14.66), the continuity equation (14.69) contains the two Laplacian terms $\square\Psi$ and $\square\phi$. Combining this equation with Eq. (14.74), the term $\square\Psi$ can be eliminated to derive a closed-form equation of ϕ . Under the approximation $e^{2\Phi} \simeq 1$, we obtain [47]

$$\square\phi \simeq \mu_4\rho + \mu_5, \quad (14.78)$$

where

$$\mu_4 = -\frac{r}{4G_4\beta} \left[2G_{4,\phi} + 4XG_{4,\phi X} - 2XG_{3,X} - \phi'\beta - \frac{4X(G_{5,X} + XG_{5,XX})}{r^2} \right], \quad (14.79)$$

$$\mu_5 = -\frac{1}{\beta r} \left[(G_{2,\phi} - 2XG_{2,\phi X} + 2XG_{3,\phi\phi})r^2 - 4X(G_{2,XX} - 2G_{3,\phi X} + 2G_{4,\phi\phi X})\phi'r \right. \\ \left. - 4X(3G_{3,X} + 4XG_{3,XX} - 9G_{4,\phi X} - 10XG_{4,\phi XX} + XG_{5,\phi\phi X}) \right. \\ \left. + \frac{8X\phi'(3G_{4,XX} + 2XG_{4,XXX} - 2G_{5,\phi X} - XG_{5,\phi XX})}{r} \right], \quad (14.80)$$

$$\beta = (G_{2,X} + 2XG_{2,XX} - 2G_{3,\phi} - 2XG_{3,\phi X})r \\ - 4\phi'(G_{3,X} + XG_{3,XX} - 3G_{4,\phi X} - 2XG_{4,\phi XX}) \\ - \frac{4X(3G_{4,XX} + 2XG_{4,XXX} - 2G_{5,\phi X} - XG_{5,\phi XX})}{r}. \quad (14.81)$$

Instead of the parameters (14.72) and (14.73), we have used original functions like $G_{3,\phi}$ in Eqs. (14.79)–(14.81).

Eliminating the term $\square\phi$ from Eqs. (14.74) and (14.78), we can derive the modified Poisson equation for Ψ as

$$\square\Psi \simeq 4\pi G_{\text{eff}}\rho + \mu_3 + \mu_2\mu_5, \quad (14.82)$$

where

$$\begin{aligned} G_{\text{eff}} &= \frac{1}{4\pi}(\mu_1 + \mu_2\mu_4) \\ &= \frac{1}{16\pi G_4} \left[1 + \frac{r}{G_4\beta} \alpha \left(\alpha - \frac{1}{2}\phi'\beta \right) + 3\Phi + \mathcal{O}(\varepsilon_i) \right], \end{aligned} \quad (14.83)$$

$$\alpha = G_{4,\phi} + 2XG_{4,\phi X} - XG_{3,X} - \frac{2X(G_{5,X} + XG_{5,XX})}{r^2}. \quad (14.84)$$

In GR ($G_4 = M_{\text{pl}}^2/2$, $G_3 = G_5 = 0$), the quantity α vanishes. The modification of gravity arises for theories characterized by

$$\alpha \neq 0. \quad (14.85)$$

In this case, the second term in the square bracket of Eq. (14.83) contributes to G_{eff} . Let us consider a non-minimal coupling to gravity arising in BD theories given by the action (11.63), i.e.,

$$G_4(\phi) = \frac{M_{\text{pl}}^2}{2} e^{-2Q\phi/M_{\text{pl}}}. \quad (14.86)$$

In this case, for the functions $G_2 = X$ and $G_3 = G_5 = 0$, the effective gravitational coupling (14.83) reduces to $G_{\text{eff}} \simeq G\{1 + 2Q^2[1 + \phi'r/(2QM_{\text{pl}})] + 3\Phi + \mathcal{O}(\varepsilon_i)\}$ for $|\phi/M_{\text{pl}}| \ll 1$. Then, the deviation of G_{eff} from G is significant due to the presence of the term $2Q^2$. In Sec. 14.1, we employed the chameleon mechanism for suppressing fifth forces mediated by the scalar field ϕ .

The Vainshtein mechanism [3], which is based on non-linear field derivative interactions like $X\square\phi$, can also allow the screening of fifth forces even in the presence of the non-minimal coupling (14.86). In the DGP braneworld [34], such derivative couplings arise for a longitudinal graviton ϕ together with the non-minimal coupling (14.86) on the brane [35, 36]. As we will see below, the derivative interactions appearing in μ_5 dominate over the matter coupling term $\mu_4\rho$ within a so-called Vainshtein radius r_V . This leads to an effective decoupling of the field ϕ with the matter sector.

Since the Vainshtein mechanism can be at work without the field potential $V(\phi)$, we consider the purely k-essence Lagrangian in the form $G_2 = g_2(X)$. For the functions G_3, G_4, G_5 , we consider derivative couplings described by the functions $g_i(X)$ with the non-minimal coupling (14.86). In summary, we focus on theories given by the functions

$$G_2 = g_2(X), \quad G_3 = g_3(X), \quad G_4 = \frac{M_{\text{pl}}^2}{2} e^{-2Q\phi/M_{\text{pl}}} + g_4(X), \quad G_5 = g_5(X). \quad (14.87)$$

The covariant Galileon (11.165) corresponds to the choices $g_2(X) \propto X$, $g_3(X) \propto X$, $g_4(X) \propto X^2$, $g_5(X) \propto X^2$ with $Q = 0$. The above theories are the generalization of covariant Galileons in which the coupling Q is present. In principle the functions (14.87) can be further generalized to contain the ϕ dependence like $G_i = e^{-\lambda_i \phi / M_{\text{Pl}}} g_i(X)$, but the resulting solutions in such models are similar to those derived for the functions (14.87) [47].

14.2.2. General arguments for field profiles

Before entering specific models, we provide general arguments for the field profile around a compact object with radius r_s by assuming that the coupling Q is of the order of unity. The matter density ρ is a general function of r . There are three distinct regimes of solutions: (A) $r > r_V$, (B) $r_s < r < r_V$, and (C) $r < r_s$, where r_V is the Vainshtein radius in which field derivative interactions suppress the propagation of fifth forces. In Sec. 14.2.3, we consider concrete models and derive explicit forms of field profiles and gravitational potentials for $r < r_V$.

(A) $r > r_V$

Outside the Vainshtein radius, non-linear derivative interactions are suppressed in Eq. (14.78). In this regime, the term $2G_{4,\phi}$ is the dominant contribution to Eq. (14.79), i.e.,

$$|2G_{4,\phi}| \gg \left| 2XG_{3,X} + \phi' \beta + 4(G_{5,X} + XG_{5,XX}) \frac{X}{r^2} \right|. \quad (14.88)$$

We assume that the field is in the range

$$|\phi| \ll M_{\text{Pl}}, \quad (14.89)$$

which can be justified after deriving the field profile. The function $g_4(X)$ should not exceed the order of M_{Pl}^2 , i.e.,

$$\frac{M_{\text{Pl}}^2}{2} e^{-2Q\phi/M_{\text{Pl}}} \gg g_4(X). \quad (14.90)$$

We consider a canonical scalar field given by

$$G_2 = X. \quad (14.91)$$

Since field derivative couplings are suppressed for $r > r_V$, the term $G_{2,X} r$ is the dominant contribution to Eq. (14.81), i.e.,

$$r \gg \left| 4(G_{3,X} + XG_{3,XX})\phi' - 2(3G_{4,XX} + 2XG_{4,XXX}) \frac{\phi'^2}{r} \right|. \quad (14.92)$$

Outside the Vainshtein radius, the matter-coupling term $\mu_4 \rho$ dominates over the term μ_5 , such that

$$|\mu_4| \rho \gg |\mu_5|. \quad (14.93)$$

Under the above conditions we have $\mu_4 \simeq Q/M_{\text{pl}}$, so the field equation (14.78) is approximately given by

$$\frac{d}{dr}(r^2\phi') \simeq Q M_{\text{pl}} \frac{dr_g}{dr}, \quad (14.94)$$

where

$$r_g = \frac{1}{M_{\text{pl}}^2} \int_0^r \rho(\tilde{r}) \tilde{r}^2 d\tilde{r} \quad (14.95)$$

is the Schwarzschild radius of the compact object. Integrating Eq. (14.94) with respect to r , we obtain the following solution

$$\phi'(r) = \frac{Q M_{\text{pl}} r_g}{r^2}, \quad (14.96)$$

where we imposed the boundary condition $\phi'(\infty) = 0$. The scalar field mediates the fifth force with an amplitude $|Q\phi'(r)/M_{\text{pl}}| = Q^2 r_g/r^2$, which is of the same order as the Newton's gravitational force r_g/r^2 . Hence the gravitational interaction is strongly modified from that in GR for the distance $r > r_V$. Under the boundary condition $\phi(\infty) \rightarrow 0$, the integrated solution to Eq. (14.96) yields

$$\phi(r) = -\frac{Q M_{\text{pl}} r_g}{r}, \quad (14.97)$$

so that the condition (14.89) translates to $r \gg r_g$ for $|Q| = \mathcal{O}(1)$. For a given model it is necessary to confirm whether the conditions (14.88), (14.90), (14.92), and (14.93) are satisfied.

(B) $r_s < r < r_V$

For $r < r_V$, non-linear derivative interactions dominate over the matter coupling term $\mu_4\rho$ in Eq. (14.78), such that

$$|\mu_4|\rho \ll |\mu_5|. \quad (14.98)$$

We define the Vainshtein radius r_V at which field derivative interactions become comparable to the term $G_{2,X} r$ in Eq. (14.81), i.e.,

$$r_V = \left| 4(G_{3,X} + XG_{3,XX})\phi'(r_V) - 2(3G_{4,XX} + 2XG_{4,XXX}) \frac{\phi'^2(r_V)}{r_V} \right|. \quad (14.99)$$

For a given model, r_V is explicitly known by solving Eq. (14.99). We note that the opposite inequality to Eq. (14.92) holds for the distance $r < r_V$. Under the condition (14.98), the field equation (14.78) reads

$$\frac{d}{dr}(r^2\phi') \simeq \frac{r(3G_{3,X} + 4XG_{3,XX}) - 2\phi'(3G_{4,XX} + 2XG_{4,XXX})}{2r(G_{3,X} + XG_{3,XX}) - \phi'(3G_{4,XX} + 2XG_{4,XXX})} r\phi'. \quad (14.100)$$

This explicitly states that the field profile inside the Vainshtein radius is determined by derivative interactions in the functions $G_3(X)$ and $G_4(X)$. For a given model, the solution to $\phi(r)$ is known by integrating Eq. (14.100). The consistency of the condition (14.98) should be checked after deriving the solution.

(C) $r < r_s$

Since the density ρ is large inside the compact object like the Sun, the condition (14.98) tends to be violated. At the center of the body we impose the following boundary condition:

$$\phi'(0) = 0. \quad (14.101)$$

If all the derivative terms $g_{2,3,4,5}(X)$ in Eq. (14.87) are suppressed relative to the term $G_4 = M_{\text{pl}}^2 e^{-2Q\phi/M_{\text{pl}}} / 2$, the scalar field obeys the same equation as (14.94), i.e., $d(r^2 \phi')/dr \simeq Q\rho r^2/M_{\text{pl}}$. We consider the situation in which the matter density approaches a constant value ρ_c as $r \rightarrow 0$. Then, the integrated solution around $r = 0$ is given by $\phi'(r) \simeq Q\rho_c r/(3M_{\text{pl}})$, which satisfies the boundary condition (14.101). However, this solution gives rise to a significant modification of gravity around the surface of body. In other words, it does not match the exterior screened solution derived from Eq. (14.100) around $r = r_s$.

Existence of the derivative interactions leads to solutions different from $\phi'(r) \simeq Q\rho_c r/(3M_{\text{pl}})$ around the center of body. Let us consider the case in which the quantities μ_4 and μ_5 approach constant values as $r \rightarrow 0$. Then, around $r = 0$, we can integrate Eq. (14.78) to give

$$\phi'(r) = \frac{1}{3} (\mu_4 \rho_c + \mu_5) r, \quad (14.102)$$

which satisfies the boundary condition (14.101). From Eqs. (14.79) and (14.80), the terms μ_4 and μ_5 contain the field derivative $\phi'(r)$. For a given model, we can derive an explicit form of ϕ' by substituting $\phi' = \mathcal{C}r$ into Eq. (14.102) and solving it for the constant $\mathcal{C}$. If the Vainshtein mechanism is at work inside the body, the constant $\mathcal{C}$ is much smaller than the unscreened value $Q\rho_c/(3M_{\text{pl}})$ mentioned above. In such cases, two screened solutions inside and outside the body smoothly connect each other around $r = r_s$.

14.2.3. Concrete models

We consider cubic and quartic Galileon interactions to obtain concrete field profiles and gravitational potentials. We will see how the propagation of fifth forces is suppressed through the operation of the Vainshtein mechanism. In the following, we choose the function $G_2 = X$ and assume the presence of the non-minimal coupling term $M_{\text{pl}}^2 e^{-2Q\phi/M_{\text{pl}}} / 2$ in G_4 .

14.2.3.1. Cubic Galileon Lagrangian

The cubic Galileon derivative interaction is given by the function

$$G_3(X) = \frac{c_3}{M^3} X, \quad (14.103)$$

where c_3 is a dimensionless constant, and M is a constant having a dimension of mass. For its relevance to the late-time cosmic acceleration, we normalize the mass M to be $M^3 = M_{\text{pl}} H_0^2$, where H_0 is today's Hubble parameter.

For the function (14.103), Eq. (14.100) reduces to

$$\frac{d}{dr} (r^2 \phi') \simeq \frac{3}{2} r \phi', \quad (14.104)$$

which is integrated to give

$$\phi'(r) \simeq C r^{-1/2}. \quad (14.105)$$

The integration constant C is known by matching this solution with Eq. (14.96) at $r = r_V$. This gives the following solution in the regime $r_s < r < r_V$:

$$\phi'(r) = \frac{Q M_{\text{pl}} r_g}{r_V^2} \left(\frac{r}{r_V} \right)^{-1/2}. \quad (14.106)$$

The behavior of solutions changes from (14.96) to (14.106) around $r = r_V$. Inside the Vainshtein radius, the field derivative $\phi'(r)$ changes slowly compared to that for $r > r_V$. From Eq. (14.99), the Vainshtein radius can be estimated as

$$r_V = \left(\frac{4|c_3 Q| M_{\text{pl}} r_g}{M^3} \right)^{1/3} \approx (|c_3 Q| r_g H_0^{-2})^{1/3}. \quad (14.107)$$

For $|c_3|$ and $|Q|$ of the order of unity, $r_V \approx (r_g H_0^{-2})^{1/3}$. Since $H_0^{-1} \approx 10^{28}$ cm, we have $r_V \approx 10^{20}$ cm for the Sun ($r_g \approx 10^5$ cm). This radius is much larger than the solar-system scale ($\approx 10^{14}$ cm).

Now, we check the consistency of assumptions used to derive the solution (14.96) for the distance r larger than r_V . Since $g_4(X) = 0$, the condition (14.90) is automatically satisfied. The condition (14.92) simply corresponds to $r \gg r_V$, where r_V is given by Eq. (14.107). Using the solution (14.96) with $\beta \simeq r$, the condition (14.88) translates to $r \gg r_g$.

On using the solution (14.96) in the region $r > r_V$, the quantities μ_4 and μ_5 are given, respectively, by $\mu_4 \simeq Q/M_{\text{pl}}$ and $\mu_5 \simeq -6c_3(QM_{\text{pl}}r_g)^2/(M^3r^6)$. The distance r_* at which $|\mu_4\rho|$ becomes equivalent to μ_5 can be estimated as

$$r_* = \left(\frac{6|c_3 Q| M_{\text{pl}}^3 r_g^2}{M^3 \rho} \right)^{1/6}. \quad (14.108)$$

Then, the ratio between r_* and r_V reads

$$\frac{r_*}{r_V} = \left(\frac{3M^3 M_{\text{pl}}}{8|c_3 Q| \rho} \right)^{1/6} \approx \left(\frac{M_{\text{pl}}^2 H_0^2}{|c_3 Q| \rho} \right)^{1/6}. \quad (14.109)$$

Provided that the matter density ρ is not very different from the cosmological density $\rho_0 \approx M_{\text{pl}}^2 H_0^2$, r_* is of the same order as r_V for $|c_3 Q| = \mathcal{O}(1)$. Then, the solution changes from (14.96) to (14.106) around r_V ($\approx r_*$). This means that the condition (14.93) is satisfied for $r \gg r_V$.

Around the center of body, we search for the solution in the form $\phi'(r) = Cr$, where C is a constant. The quantities μ_4 and μ_5 approach the constant values $\mu_4 = QM^3/[M_{\text{pl}}(M^3 - 4c_3 C)]$ and $\mu_5 = -6c_3 C^2/(M^3 - 4c_3 C)$ as $r \rightarrow 0$, so we can employ Eq. (14.102) to solve for C . This process leads to the following solution around $r = 0$ [43]:

$$\phi'(r) = \frac{M^3}{4c_3} \left[1 - \sqrt{1 - \frac{8c_3 Q \rho_c}{3M^3 M_{\text{pl}}}} \right] r. \quad (14.110)$$

In the limit that $c_3 \rightarrow 0$, the solution (14.110) recovers the unscreened solution $\phi'(r) = Q\rho_c r/(3M_{\text{pl}})$. Existence of the coupling c_3 gives rise to a screened solution inside the body. Let us consider the case in which the condition

$$|c_3 Q| \rho_c \gg M^3 M_{\text{pl}} \quad (14.111)$$

is satisfied with

$$c_3 Q < 0. \quad (14.112)$$

In this case, Eq. (14.110) reduces to

$$\phi'(r) \simeq -\frac{1}{c_3} \sqrt{\frac{|c_3 Q| M^3 \rho_c}{6M_{\text{pl}}}} r. \quad (14.113)$$

Compared to the unscreened solution $\phi'(r) = Q\rho_c r/(3M_{\text{pl}})$, the amplitude of the solution (14.113) is suppressed by the ratio of the order $\sqrt{M^3 M_{\text{pl}}/(|c_3 Q| \rho_c)} \ll 1$.

The result (14.113) is valid around $r = 0$, but it is possible to extrapolate this solution to the surface of body by assuming that the density is nearly constant ($\simeq \rho_c$) inside the body. From Eq. (14.95), the Schwarzschild radius can be estimated as $r_g \approx \rho_c r_s^3/M_{\text{pl}}^2$. Using this relation to eliminate the density ρ_c in Eq. (14.113), the amplitude of $\phi'(r)$ around the surface of body is approximately given by

$$|\phi'_{\text{in}}(r_s)| \approx \sqrt{\frac{M^3 M_{\text{pl}} |Q| r_g}{|c_3| r_s}}. \quad (14.114)$$

On using the exterior screened solution (14.106) with r_V given by Eq. (14.107), we find that $|\phi'_{\text{out}}(r_s)|$ is the same order as $|\phi'_{\text{in}}(r_s)|$. If $c_3 > 0$ ($c_3 < 0$), then Q is negative (positive) and hence the sign of Eq. (14.106) is the same as that

of Eq. (14.113). Hence the two screened solutions (14.106) and (14.113) smoothly match with each other around $r = r_s$.

Let us derive corrections to Newtonian gravitational potentials by using the screened solution (14.106) for the distance $r_s < r < r_V$. The dominant contributions to Eqs. (14.65) and (14.66) correspond to those containing the term G_4 and its ϕ derivatives, such that

$$\frac{4G_4}{r}\Phi' + \frac{4G_4}{r^2}\Phi - 2G_{4,\phi}\phi'' - \frac{4G_{4,\phi}}{r}\phi' - 2G_{4,\phi\phi}\phi'^2 \simeq \rho, \quad (14.115)$$

$$\frac{4G_4}{r}\Psi' - \frac{4G_4}{r^2}\Phi + \frac{4G_{4,\phi}}{r}\phi' \simeq 0. \quad (14.116)$$

Substituting the solution (14.106) into Eq. (14.115), it follows that the last term on the left hand side is subdominant to other terms and hence

$$\frac{d}{dr} \left(r\Phi - \frac{r_g}{2} \right) \simeq -\frac{3Q^2 r_g r^{1/2}}{2r_V^{3/2}}. \quad (14.117)$$

This is integrated to give

$$\Phi(r) \simeq \frac{r_g}{2r} \left[1 - 2Q^2 \left(\frac{r}{r_V} \right)^{3/2} \right], \quad (14.118)$$

where the integration constant has been absorbed into the definition of r_g given by Eq. (14.95). On using the solution (14.118), we can integrate Eq. (14.116) to give

$$\Psi(r) \simeq -\frac{r_g}{2r} \left[1 - 4Q^2 \left(\frac{r}{r_V} \right)^{3/2} \right]. \quad (14.119)$$

For the distance $r \ll r_V$, the second terms inside the square brackets of Eqs. (14.118) and (14.119) are much smaller than unity, so the corrections to leading-order gravitational potentials are suppressed under the operation of the Vainshtein mechanism. Since the post-Newtonian parameter $\gamma = -\Phi/\Psi$ can be estimated as $\gamma \simeq 1 + 2Q^2(r/r_V)^{3/2}$, the local gravity constraint (14.44) translates to

$$Q^2 \left(\frac{r}{r_V} \right)^{3/2} < 1.2 \times 10^{-5}. \quad (14.120)$$

For the Sun, the Vainshtein radius is of the order of 10^{20} cm for $|Q|$ and $|c_3|$ of the order of 1. Hence the bound (14.120) is well satisfied inside the solar-system scale ($r \lesssim 10^{14}$ cm). Thus, the Vainshtein mechanism induced by the cubic Galileon term allows the screening of fifth forces in the solar system.

14.2.3.2. Quartic Galileon Lagrangian

Let us proceed to the Galileon model with quartic derivative interactions given by

$$g_4(X) = \frac{c_4}{M^6} X^2, \quad (14.121)$$

where c_4 is a constant, and the mass M satisfies the normalization $M^3 = M_{\text{pl}} H_0^2$. In this case, the field equation (14.100) yields

$$\frac{d}{dr} (r^2 \phi') \simeq 2r \phi', \quad (14.122)$$

whose solution is simply given by

$$\phi'(r) = C, \quad (14.123)$$

where C is a constant. Matching this with (14.96) at $r = r_V$, the solution for the distance $r_s < r < r_V$ yields

$$\phi'(r) = \frac{Q M_{\text{pl}} r_g}{r_V^2}. \quad (14.124)$$

From Eq. (14.99), the Vainshtein radius can be estimated as

$$r_V = \left(\frac{12|c_4|Q^2 M_{\text{pl}}^2 r_g^2}{M^6} \right)^{1/6} \approx (|c_4 Q^2|)^{1/6} (r_g H_0^{-2})^{1/3}. \quad (14.125)$$

For $|c_4|$ and $|Q|$ of the order of 1, we obtain the Vainshtein radius $r_V \approx (r_g H_0^{-2})^{1/3}$ same as that derived for the cubic Galileon. On using the solution (14.96), the distance r_* at which $|\mu_4 \rho|$ is equivalent to $|\mu_5|$ is given by $r_* = [24|c_4|Q^2 M_{\text{pl}}^4 r_g^3 / (M^6 \rho)]^{1/9}$. Then we obtain the ratio $r_*/r_V \approx [M^3 M_{\text{pl}} / (|c_4|^{1/2} |Q| \rho)]^{1/9} = [M_{\text{pl}}^2 H_0^2 / (|c_4|^{1/2} |Q| \rho)]^{1/9}$. As long as ρ is close to the cosmological density ρ_0 , r_* is of the same order as r_V . Hence the condition (14.93) used for the derivation of the solution (14.96) is satisfied for $r \gg r_V$. As in the case of cubic Galileons, we can confirm that other conditions (14.88), (14.90), (14.92) are also satisfied for $r \gg r_V \gg r_g$.

Around the center of body, we are searching for the solution in the form $\phi'(r) = \mathcal{C}r$, so that $\mu_4 = Q M^6 / [M_{\text{pl}} (M^6 + 12c_4 \mathcal{C}^2)]$ and $\mu_5 = 24c_4 \mathcal{C}^3 / (M^6 + 12c_4 \mathcal{C}^2)$ as $r \rightarrow 0$. In the limit that $c_4 \rightarrow 0$, Eq. (14.102) recovers the unscreened solution $\phi'(r) = Q \rho_c r / (3M_{\text{pl}})$. In another limit $c_4 \mathcal{C}^2 \gg M^6$, we obtain the following screened solution

$$\phi'(r) \simeq \left(\frac{Q M^6 \rho_c}{12 M_{\text{pl}} c_4} \right)^{1/3} r. \quad (14.126)$$

To match this solution with (14.124) around the surface of body, we require that

$$c_4 > 0. \quad (14.127)$$

Extrapolating the solution (14.126) to the surface of body, the amplitude of $\phi'(r)$ can be estimated as

$$|\phi'_{\text{in}}(r_s)| \approx \left(\frac{M^6 M_{\text{pl}} |Q| r_g}{c_4} \right)^{1/3}. \quad (14.128)$$

On using the exterior solution (14.124), the field derivative $|\phi'_{\text{out}}(r_s)|$ is of the same order as the right hand side of Eq. (14.128). Hence the two screened solutions (14.124) and (14.128) smoothly match with each other around $r = r_s$.

We have studied the case in which the density is nearly constant inside the body, but the above result is also valid for the r -dependent density profile $\rho(r)$. For concreteness, we consider the density profile

$$\rho(r) = \rho_c e^{-r^2/r_t^2}, \quad (14.129)$$

where r_t is the transition radius at which $\rho(r)$ starts to decrease significantly. For the numerical purpose, we define the dimensionless quantities

$$y = \frac{M_{\text{pl}} \phi'^3(r)}{M^6 \rho_c r_s^3}, \quad \lambda_1 = \left(\frac{\rho_c r_s^2}{M_{\text{pl}}^2} \right)^{1/3}, \quad \lambda_2 = \left(\frac{M^3 r_s^2}{M_{\text{pl}}} \right)^{1/3}, \quad (14.130)$$

and $x = r/r_s$ and $z = \phi/M_{\text{pl}}$. In Fig. 14.3, we plot $y^{1/3}$ versus r/r_s for $\lambda_1 = 0.1$, $\lambda_2 = 3 \times 10^{-12}$, $Q = 1$, $c_4 = 1$, and $r_t/r_s = 0.5$. The parameters λ_1 and λ_2 are chosen

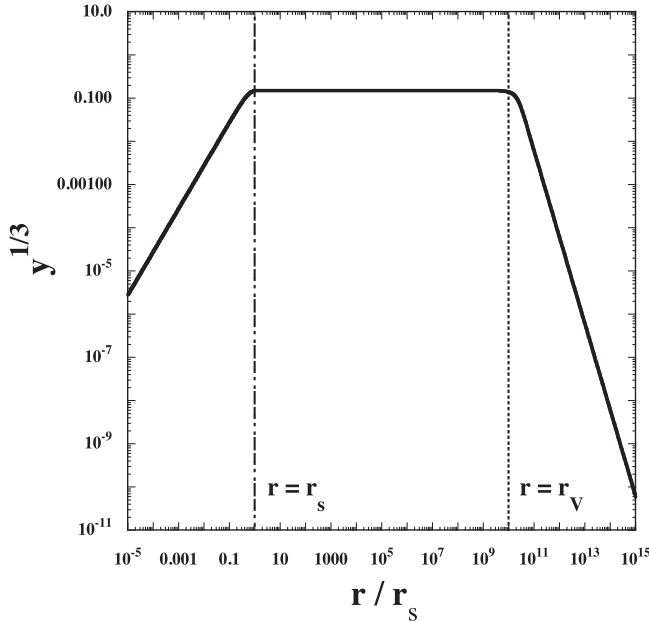


Fig. 14.3. The dimensionless field derivative $y^{1/3} = [M_{\text{pl}}/(M^6 \rho_c r_s^3)]^{1/3} \phi'(r)$ versus r/r_s for $Q = 1$, $\lambda_1 = 0.1$, $\lambda_2 = 3.0 \times 10^{-12}$, $r_t = 0.5r_s$, and $c_4 = 1$ with the density profile (14.129). We also plot two radii $r = r_s$ and $r = r_V$ as vertical lines.

to mimic those of the Sun ($\rho_c \simeq 100 \text{ g/cm}^3$ and $r_s \simeq 7 \times 10^{10} \text{ cm}$). Numerically we integrate Eq. (14.78) with $dz/dx = \lambda_1 \lambda_2^2 y^{1/3}$ to obtain $\phi'(r)$ and $\phi(r)$. For $r \ll r_s$ the field derivative $\phi'(r)$ linearly grows in r according to Eq. (14.126). Around $r = r_s$, it matches another screened solution (14.124). The field derivative stays nearly constant in the region $r_s < r < r_V$, but, for $r > r_V$, it starts to decrease rapidly as Eq. (14.96). Thus the Vainshtein mechanism is at work to suppress the propagation of fifth forces for $r < r_V$.

As in the case of cubic Galileons, the gravitational potentials obey the approximate equations (14.115) and (14.116). On using the solution (14.124), the integrated solutions to Φ and Ψ are given, respectively, by

$$\Phi(r) \simeq \frac{r_g}{2r} \left[1 - 2Q^2 \left(\frac{r}{r_V} \right)^2 \right], \quad (14.131)$$

$$\Psi(r) \simeq -\frac{r_g}{2r} \left[1 - 2Q^2 \left(\frac{r}{r_V} \right)^2 \right]. \quad (14.132)$$

Hence the post-Newtonian parameter $\gamma = -\Phi/\Psi$ reduces to $\gamma \simeq 1$. The deviation of γ from 1 arises only from terms higher than $2Q^2(r/r_V)^2$. Hence the local gravity constraint (14.44) is well satisfied in the solar system.

In the presence of quintic derivative interactions like $G_5(X) = c_5 X^2/M^9$ with $c_5 > 0$, the success of the Vainshtein mechanism induced by the quartic interaction $g_4(X) = c_4 X^2/M^6$ tends to break down for small radius [44]. This is not the case for $c_5 < 0$, in which the field derivative $\phi'(r)$ is subject to a stronger suppression relative to the case $c_5 = 0$ [47, 48]. We note that the covariant Galileon given by the action (11.165) corresponds to $Q \rightarrow 0$, so the field derivative $\phi'(r)$ vanishes. Hence the propagation of fifth forces is even more suppressed in such a limit.

14.3. Vainshtein mechanism in generalized Proca theories

In Chap. 13, we studied the cosmology in generalized Proca theories given by the action (13.31). Derivative interactions of the vector field A^μ allow the existence of de Sitter solutions relevant to the late-time cosmic acceleration. Now, we are interested in whether such derivative interactions can lead to the suppression of fifth forces in local regions of the Universe. The Vainshtein mechanism in generalized Proca theories was addressed in Refs. [49, 52]. For concreteness, we consider quartic-order generalized Proca theories given by the action

$$\begin{aligned} S = \int d^4x \bigg[& \sqrt{-g} \{ G_2(X) + G_3(X) \nabla_\mu A^\mu \\ & + G_4(X) R + G_{4,X}(X) [(\nabla_\mu A^\mu)^2 - \nabla_\rho A_\sigma \nabla^\sigma A^\rho] \} + L_m(g_{\mu\nu}, \Psi_m) \bigg], \end{aligned} \quad (14.133)$$

where L_m is the Lagrangian of matter fields Ψ_m . We assume that the matter sector is described by a perfect fluid (density ρ and pressure P) minimally coupled to gravity.

Unlike Horndeski theories in which the scalar field ϕ is coupled to the Ricci scalar R in the form $G_4(\phi, X)R$, the function G_4 has only the dependence of $X = -A_\mu A^\mu/2$. Hence non-minimal couplings like (14.86) are absent in generalized Proca theories. Still, the quantity X contains both the temporal component ϕ and the derivative of a longitudinal mode χ , so it is of interest to see how they gravitate around a compact object. In the quadratic term G_2 it is possible to take into account the dependence of $F = -F_{\mu\nu}F^{\mu\nu}/4$ etc, but the existence of such an intrinsic vector mode does not substantially modify the discussion of the Vainshtein mechanism given below [49].

We consider the spherically symmetric and static background described by the line element (14.64). First, the perfect fluid satisfies the continuity equation (14.69). We express the vector field A^μ in the form

$$A^\mu = (\phi, A^i), \quad (14.134)$$

where $i = 1, 2, 3$. The spatial components A^i can be decomposed into transverse and longitudinal modes, as

$$A_i = A_i^{(T)} + \nabla_i \chi, \quad (14.135)$$

where $A_i^{(T)}$ obeys the transverse condition $\nabla^i A_i^{(T)} = 0$ and χ is the longitudinal scalar field. The θ and φ components of $A_i^{(T)}$ need to vanish on the spherically symmetric and static background. From the transverse condition the radial component $A_1^{(T)}$ obeys

$$A_1^{(T)'} + \frac{2}{r}A_1^{(T)} - \Phi' A_1^{(T)} = 0, \quad (14.136)$$

where a prime represents a derivative with respect to r . The integrated solution to this equation is given by

$$A_1^{(T)} = \mathcal{C} \frac{e^\Phi}{r^2}, \quad (14.137)$$

where $\mathcal{C}$ is a constant. To avoid the divergence of $A_1^{(T)}$ at $r = 0$, we require that $\mathcal{C} = 0$. Since the transverse vector field $A_i^{(T)}$ vanishes, we only need to focus on the propagation of the longitudinal mode, i.e., $A_i = \nabla_i \chi$. Hence the components of A^μ on the coordinate (t, r, θ, φ) can be expressed as

$$A^\mu = (\phi(r), e^{-2\Phi} \chi'(r), 0, 0). \quad (14.138)$$

The action (14.133) can be expressed in terms of ϕ, χ and Ψ, Φ by employing Eq. (14.138) with the line element (14.64). Varying the action with respect to ϕ and

χ , the resulting vector equations of motion are given, respectively, by [49]

$$2\phi(\Psi'\Phi' - \Psi'' - \Psi'^2) + \left[\phi\chi'G_{3,X} - 3\phi' - \frac{4\phi}{r}(1 + 2X_\chi G_{4,XX}) \right] \Psi' + e^{2\Phi}\phi G_{2,X} \\ + \phi\chi''G_{3,X} - \phi'' + \left[\phi' - \phi\chi'G_{3,X} + \frac{4\phi}{r}(G_{4,X} + 2X_\chi G_{4,XX}) \right] \Phi' + \frac{1}{r}(2\phi\chi'G_{3,X} \\ - 2\phi' + 4e^{-2\Phi}\phi\chi'\chi''G_{4,XX}) - \frac{2\phi}{r^2}[(1 - e^{2\Phi})G_{4,X} + 2X_\chi G_{4,XX}] = 0, \quad (14.139)$$

$$\left[2(X_\chi - X_\phi)G_{3,X} + \frac{4e^{-2\Phi}\chi'}{r}\{G_{4,X} + 2(X_\chi - X_\phi)G_{4,XX}\} \right] \Psi' \\ - \chi'G_{2,X} - e^{2\Psi}\phi\phi'G_{3,X} + \frac{4}{r}(X_\chi G_{3,X} - e^{2\Psi-2\Phi}\phi\phi'\chi'G_{4,XX}) \\ - \frac{2\chi'}{r^2}[(1 - e^{-2\Phi})G_{4,X} - 2e^{-2\Phi}X_\chi G_{4,XX}] = 0, \quad (14.140)$$

where $X = X_\phi + X_\chi$ with

$$X_\phi = \frac{1}{2}e^{2\Psi}\phi^2, \quad X_\chi = -\frac{1}{2}e^{-2\Phi}\chi'^2. \quad (14.141)$$

Variation of the action (14.133) with respect to Ψ and Φ leads to

$$\mathcal{C}_1\Psi'^2 + \left(\mathcal{C}_2 + \frac{\mathcal{C}_3}{r}\right)\Psi' + \left(\mathcal{C}_4 + \frac{\mathcal{C}_5}{r}\right)\Phi' + \mathcal{C}_6 + \frac{\mathcal{C}_7}{r} + \frac{\mathcal{C}_8}{r^2} = -e^{2\Phi}\rho, \quad (14.142)$$

$$\mathcal{C}_9\Psi'^2 + \left(\mathcal{C}_{10} + \frac{\mathcal{C}_{11}}{r}\right)\Psi' + \mathcal{C}_{12} + \frac{\mathcal{C}_{13}}{r} + \frac{\mathcal{C}_{14}}{r^2} = e^{2\Phi}P, \quad (14.143)$$

where

$$\mathcal{C}_1 = 4X_\phi, \quad \mathcal{C}_2 = 4\chi'X_\phi G_{3,X} + 2e^{2\Psi}\phi\phi', \\ \mathcal{C}_3 = -32X_\phi X_\chi G_{4,XX}, \quad \mathcal{C}_4 = -2\chi'(X_\phi + X_\chi)G_{3,X}, \\ \mathcal{C}_5 = -4[G_4 - 2(X_\phi + 2X_\chi)G_{4,X} - 4X_\chi(X_\phi + X_\chi)G_{4,XX}], \\ \mathcal{C}_6 = -e^{2\Phi}(G_2 - 2X_\phi G_{2,X}) + [e^{2\Psi}\phi\phi'\chi' + 2\chi''(X_\phi + X_\chi)]G_{3,X} + \frac{1}{2}e^{2\Psi}\phi'^2, \\ \mathcal{C}_7 = 4\chi'X_\phi G_{3,X} + 4e^{-2\Phi}\chi'\chi''G_{4,X} + 8[e^{-2\Phi}\chi'\chi''(X_\phi + X_\chi) - e^{2\Psi}\phi\phi'X_\chi]G_{4,XX}, \\ \mathcal{C}_8 = 2(1 - e^{2\Phi})G_4 - 4[X_\chi + (1 - e^{2\Phi})X_\phi]G_{4,X} - 8X_\phi X_\chi G_{4,XX}, \\ \mathcal{C}_9 = 4X_\phi, \quad \mathcal{C}_{10} = 2\chi'(X_\chi - X_\phi)G_{3,X} + 2e^{2\Psi}\phi\phi', \\ \mathcal{C}_{11} = 4[G_4 + 2(X_\phi - 2X_\chi)G_{4,X} + 4X_\chi(X_\phi - X_\chi)G_{4,XX}], \\ \mathcal{C}_{12} = -e^{2\Phi}(G_2 - 2X_\chi G_{2,X}) - e^{2\Psi}\phi\phi'\chi'G_{3,X} + \frac{1}{2}e^{2\Psi}\phi'^2, \\ \mathcal{C}_{13} = 4\chi'X_\chi G_{3,X} + 4e^{2\Psi}\phi\phi'(G_{4,X} + 2X_\chi G_{4,XX}), \\ \mathcal{C}_{14} = 2(1 - e^{2\Phi})G_4 - 4X_\chi(2 - e^{2\Phi})G_{4,X} - 8X_\chi^2 G_{4,XX}. \quad (14.144)$$

We consider a compact object (radius r_s) whose density is approximately a constant ρ_0 inside the body and 0 outside the body, i.e., $\rho(r) = \rho_0$ for $r < r_s$ and $\rho(r) = 0$ for $r > r_s$. In this case, the integrated solution to Eq. (14.69) is given by $P(r) = -\rho_0 + Ce^{-\Psi(r)}$ inside the body. The integration constant C is known by the boundary condition $P(r_s) = 0$, so that

$$P(r) = \begin{cases} \rho_0(e^{\Psi(r_s)-\Psi(r)} - 1) & \text{for } r < r_s, \\ 0 & \text{for } r > r_s. \end{cases} \quad (14.145)$$

In GR without the vector field, i.e., $G_2 = G_3 = 0$, $G_4 = M_{\text{pl}}^2/2$ and $\phi = 0 = \chi'$, the gravitational Eqs. (14.142) and (14.143) reduce to Eqs. (14.70) and (14.71), respectively. Substituting Eq. (14.145) into Eqs. (14.70)–(14.71) and matching interior and exterior solutions at $r = r_s$, the resulting Schwarzschild interior and exterior solutions are given, respectively, by

$$e^{\Psi_{\text{GR}}} = \frac{3}{2} \sqrt{1 - \frac{\rho_0 r_s^2}{3M_{\text{pl}}^2}} - \frac{1}{2} \sqrt{1 - \frac{\rho_0 r^2}{3M_{\text{pl}}^2}}, \quad e^{\Phi_{\text{GR}}} = \left(1 - \frac{\rho_0 r^2}{3M_{\text{pl}}^2}\right)^{-1/2}, \quad (14.146)$$

for $r < r_s$, and

$$e^{\Psi_{\text{GR}}} = \left(1 - \frac{\rho_0 r_s^3}{3M_{\text{pl}}^2 r}\right)^{1/2}, \quad e^{\Phi_{\text{GR}}} = \left(1 - \frac{\rho_0 r_s^3}{3M_{\text{pl}}^2 r}\right)^{-1/2}, \quad (14.147)$$

for $r > r_s$. In the rest of this section, we employ the weak gravity approximation under which $|\Psi|$ and $|\Phi|$ are much smaller than 1, such that

$$\Phi_* \equiv \frac{\rho_0 r_s^2}{M_{\text{pl}}^2} \ll 1. \quad (14.148)$$

The Schwarzschild radius of the source is of the order of $r_g \approx \rho_0 r_s^3 / M_{\text{pl}}^2$, which is much smaller than r_s under the condition (14.148). In this case, Eqs. (14.146) and (14.147) reduce, respectively, to

$$\Psi_{\text{GR}} \simeq \frac{\rho_0}{12M_{\text{pl}}^2} (r^2 - 3r_s^2), \quad \Phi_{\text{GR}} \simeq \frac{\rho_0 r^2}{6M_{\text{pl}}^2}, \quad (14.149)$$

for $r < r_s$, and

$$\Psi_{\text{GR}} \simeq -\frac{\rho_0 r_s^3}{6M_{\text{pl}}^2 r}, \quad \Phi_{\text{GR}} \simeq \frac{\rho_0 r_s^3}{6M_{\text{pl}}^2 r}, \quad (14.150)$$

for $r > r_s$.

In generalized Proca theories, the vector field interacts with gravity through the derivative terms Ψ'', Ψ', Φ' in Eqs. (14.139) and (14.140). Provided that the Vainshtein mechanism allows the recovery of solutions close to those of GR, the leading-order gravitational interactions correspond to the derivatives $\Psi''_{\text{GR}}, \Psi'_{\text{GR}}, \Phi'_{\text{GR}}$ of Eqs. (14.149) and (14.150). After the substitution of such derivative terms, the

leading-order solutions to ϕ and χ' can be derived by integrating Eqs. (14.149) and (14.150). Substituting such vector field solutions into Eqs. (14.142) and (14.143), we can estimate next-to-leading order corrections to Ψ and Φ .

14.3.1. Cubic vector Galileons

Let us begin with the cubic vector Galileon given by the functions

$$G_2(X) = m^2 X, \quad G_3(X) = \beta_3 X, \quad G_4(X) = \frac{M_{\text{pl}}^2}{2}, \quad (14.151)$$

where m^2 is the mass squared of the vector field (which can be either positive or negative), and β_3 is a dimensionless constant. The function $G_4(X)$ does not have the X dependence, but the cubic term $G_3(X) = \beta_3 X$ can give rise to a non-trivial gravitational interaction with the vector field. For the model (14.151), Eqs. (14.139) and (14.140) reduce, respectively, to

$$\begin{aligned} \frac{1}{r^2} \frac{d}{dr} (r^2 \phi') - m^2 e^{2\Phi} \phi - \beta_3 \phi \frac{1}{r^2} \frac{d}{dr} (r^2 \chi') + 2\phi (\Psi'' + \Psi'^2 - \Psi' \Phi') \\ - \left(\beta_3 \phi \chi' - 3\phi' - \frac{4\phi}{r} \right) \Psi' + (\beta_3 \phi \chi' - \phi') \Phi' = 0, \end{aligned} \quad (14.152)$$

$$m^2 \chi' + \beta_3 \left[\left(e^{2\Psi} \phi \phi' + \frac{2}{r} e^{-2\Phi} \chi'^2 \right) + (e^{2\Psi} \phi^2 + e^{-2\Phi} \chi'^2) \Psi' \right] = 0. \quad (14.153)$$

Since we are interested in the case where the same model is relevant to the late-time cosmic acceleration ($m^2 \lesssim H_0^2$), we take the limit $m^2 \rightarrow 0$ for the derivation of vector-field profiles in the following.

14.3.1.1. Vector field profiles for $r < r_s$

For $r < r_s$, we can derive leading-order solutions to ϕ and χ' by substituting Eq. (14.149) into Eqs. (14.152) and (14.153). The terms containing $e^{2\Psi}$ and $e^{-2\Phi}$ give rise to the contributions linear in Ψ and Φ , but after deriving solutions to ϕ and χ' , we can show that their contributions are much smaller than leading-order solutions. On using the approximations $e^{2\Psi} \simeq 1$ and $e^{-2\Phi} \simeq 1$ in Eqs. (14.152) and (14.153), it follows that

$$\frac{d}{dr} (r^2 \phi') - \beta_3 \phi \frac{d}{dr} (r^2 \chi') + \frac{\rho_0}{6M_{\text{pl}}^2} [6\phi + r(\phi' + \beta_3 \chi' \phi)] r^2 \simeq 0, \quad (14.154)$$

$$\chi' \simeq \sqrt{-\frac{r}{2} \left(\phi \phi' + \frac{\rho_0 \phi^2}{6M_{\text{pl}}^2} r \right)}, \quad (14.155)$$

where, in Eq. (14.155), we have chosen the positive sign. If we take into account a non-vanishing mass term m , we can also obtain the solution (14.155) by taking the

limit $\beta_3/m^2 \rightarrow \infty$ with $\beta_3 > 0$. We require that $\phi\phi' < 0$ for the consistency of the solution (14.155).

We search for solutions where the temporal vector component stays nearly constant, such that

$$\phi(r) = \phi_0 + f(r), \quad |f(r)| \ll |\phi_0|, \quad (14.156)$$

where ϕ_0 is a constant and $f(r)$ is a function of r . We also focus on the case in which $\phi(r)$ decreases as a function of r , i.e., $\phi'(r) < 0$ with $\phi_0 > 0$. We employ the approximation that the terms $r(\phi' + \beta_3\chi'\phi)$ are neglected relative to 6ϕ in Eq. (14.154), whose validity can be checked after deriving field profiles. Substituting Eq. (14.155) into Eq. (14.154) under the assumption (14.156), we obtain the integrated solution

$$f' - \beta_3\phi_0^{3/2} \sqrt{-\frac{r}{2} \left(f' + \frac{\rho_0\phi_0 r}{6M_{\text{pl}}^2} \right) + \frac{\rho_0\phi_0}{3M_{\text{pl}}^2} r} = 0, \quad (14.157)$$

where the integration constant is chosen to satisfy the boundary condition $\phi'(0) = 0$. There is the solution in the form $f(r) = -Cr^2$ (C is a positive constant), i.e., $f'(r) \propto -r$. Substituting this into Eq. (14.157), we obtain

$$C = \frac{\rho_0\phi_0}{6M_{\text{pl}}^2} \mathcal{F}(s_{\beta_3}), \quad (14.158)$$

where

$$s_{\beta_3} \equiv \frac{3(\beta_3\phi_0 M_{\text{pl}})^2}{4\rho_0}, \quad (14.159)$$

$$\mathcal{F}(s_{\beta_3}) \equiv (1 + s_{\beta_3}) \left(1 - \sqrt{\frac{s_{\beta_3}}{1 + s_{\beta_3}}} \right). \quad (14.160)$$

Then, the field profiles are given by

$$\phi(r) = \phi_0 \left[1 - \mathcal{F}(s_{\beta_3}) \frac{\rho_0}{6M_{\text{pl}}^2} r^2 \right], \quad (14.161)$$

$$\chi(r) = \sqrt{\frac{\rho_0\phi_0^2}{6M_{\text{pl}}^2} \left[\mathcal{F}(s_{\beta_3}) - \frac{1}{2} \right]} r. \quad (14.162)$$

As s_{β_3} grows from 0 to ∞ , the function $\mathcal{F}(s_{\beta_3})$ decreases from 1 to $1/2$. Hence the terms inside the square root of Eq. (14.162) remains positive. Since $\mathcal{F}(s_{\beta_3})\rho_0 r^2/(6M_{\text{pl}}^2) \ll 1$ under the weak gravity condition (14.148), the solution (14.161) is consistent with the assumption (14.156). From Eqs. (14.161) and (14.162), we can also confirm that the terms $r(\phi' + \beta_3\chi'\phi)$ in Eq. (14.154) is much smaller than 6ϕ and that the approximations $e^{2\Psi} \simeq 1$ and $e^{-2\Phi} \simeq 1$ are also justified.

If $s_{\beta_3} \ll 1$, then Eqs. (14.161) and (14.162) reduce, respectively, to

$$\phi(r) \simeq \phi_0 \left(1 - \frac{\rho_0}{6M_{\text{pl}}^2} r^2 \right), \quad \chi'(r) \simeq \sqrt{\frac{\rho_0 \phi_0^2}{12M_{\text{pl}}^2}} r, \quad (14.163)$$

whereas, for $s_{\beta_3} \gg 1$, we have

$$\phi(r) \simeq \phi_0 \left(1 - \frac{\rho_0}{12M_{\text{pl}}^2} r^2 \right), \quad \chi'(r) \simeq \frac{\rho_0}{6\beta_3 M_{\text{pl}}^2} r. \quad (14.164)$$

The amplitude of $\chi'(r)$ in Eq. (14.164) is about $s_{\beta_3}^{-1/2}$ times as small as that in Eq. (14.163). For larger $|\beta_3|$, the suppression of the longitudinal mode tends to be more efficient.

14.3.1.2. Vector field profiles for $r > r_s$

For the distance $r > r_s$, we substitute the gravitational potentials (14.150) of GR into Eqs. (14.152) and (14.153). Taking the branch $\chi' > 0$, it follows that

$$\frac{d}{dr}(r^2 \phi') - \beta_3 \phi \frac{d}{dr}(r^2 \chi') + \frac{\rho_0 r_s^3}{9M_{\text{pl}}^4 r^2} [\rho_0 r_s^3 \phi + 3M_{\text{pl}}^2 r^2 (2\phi' - \beta_3 \chi' \phi)] \simeq 0, \quad (14.165)$$

$$\chi' = \sqrt{-\frac{r}{2} \left(\phi \phi' + \frac{\rho_0 \phi^2 r_s^3}{6M_{\text{pl}}^2 r^2} \right)}. \quad (14.166)$$

In Eq. (14.165), the term $(\rho_0 r_s^3)^2 \phi / (9M_{\text{pl}}^4 r^2)$ is at most Φ_* times as small as the term $\rho_0 \phi / M_{\text{pl}}^2$ appearing in Eq. (14.154). Moreover, after deriving field profiles, we can show that the contributions $3M_{\text{pl}}^2 r^2 (2\phi' - \beta_3 \chi' \phi)$ in Eq. (14.165) is at most of the order of $\rho_0 r_s^3 \phi$. Then, we can employ an approximation to neglect the terms inside the square bracket of Eq. (14.165) relative to other terms. Plugging Eq. (14.166) into Eq. (14.165) under the approximation (14.156) and matching the integrated solution at $r = r_s$, it follows that

$$r^2 \phi' - \beta_3 \phi_0^{3/2} r^2 \sqrt{-\frac{r}{2} \left(\phi' + \frac{\rho_0 \phi_0 r_s^3}{6M_{\text{pl}}^2 r^2} \right)} \simeq -\frac{\rho_0 \phi_0 r_s^3}{3M_{\text{pl}}^2}. \quad (14.167)$$

We can explicitly solve this equation for ϕ' as

$$\phi'(r) = -\frac{\rho_0 \phi_0 r_s^3}{3M_{\text{pl}}^2 r^2} \mathcal{F}(\xi), \quad \xi \equiv s_{\beta_3} \frac{r^3}{r_s^3}. \quad (14.168)$$

From Eq. (14.166), the longitudinal mode yields

$$\chi'(r) = \sqrt{\frac{\rho_0 r_s^3 \phi_0^2}{6M_{\text{pl}}^2 r} \left[\mathcal{F}(\xi) - \frac{1}{2} \right]}. \quad (14.169)$$

If $s_{\beta_3} \gg 1$, then we have $\xi \gg 1$, so the solutions (14.168) and (14.169) reduce, respectively, to

$$\phi'(r) \simeq -\frac{\rho_0 \phi_0 r_s^3}{6M_{\text{pl}}^2 r^2}, \quad \chi'(r) \simeq \frac{\rho_0 r_s^3}{6\beta_3 M_{\text{pl}}^2 r^2}. \quad (14.170)$$

In this case, the longitudinal mode $\chi'(r)$ is strongly suppressed both outside and inside the body.

If $s_{\beta_3} \lesssim 1$, there is the transition radius r_V at which the radial dependence of $\chi'(r)$ changes. The radius r_V can be identified by the condition $\xi = 1$, i.e.,

$$r_V = \frac{r_s}{s_{\beta_3}^{1/3}}. \quad (14.171)$$

For the distance $r_s < r < r_V$ we have $\mathcal{F} \simeq 1$, so the solutions reduce to

$$\phi'(r) \simeq -\frac{\rho_0 \phi_0 r_s^3}{3M_{\text{pl}}^2 r^2}, \quad \chi'(r) \simeq \sqrt{\frac{\rho_0 r_s^3 \phi_0^2}{12M_{\text{pl}}^2 r}}. \quad (14.172)$$

For the distance $r \gg r_V$ we have $\xi \gg 1$, so the resulting solutions are given by Eq. (14.170). In this regime, $\chi'(r)$ decreases faster relative to the solution (14.172). The distance r_V may be regarded as the Vainshtein radius above which $\chi'(r)$ starts to decrease quickly. The fact that the suppression of $\chi'(r)$ occurs for $r > r_V$ is a unique feature for vector Galileons.

The analytic solutions given above have been derived by assuming $\rho(r) = \rho_0$ for $r < r_s$ and $\rho(r) = 0$ for $r > r_s$, but they do not lose the validity for r -dependent density profiles like Eq. (14.129). To see this, we numerically solve Eqs. (14.139) and (14.140) with Eqs. (14.142) and (14.143) for the density profile (14.129). In Fig. 14.4, we plot the field profiles for $r_t = r_s/2$ and $\Phi_* = 10^{-4}$ with $s_{\beta_3} = 10^{-4}$ and $s_{\beta_3} = 1$. For $r < r_s$, both $-\phi'(r)$ and $\chi'(r)$ linearly grow in r . As estimated by Eqs. (14.163) and (14.164), the amplitude of $|\chi'(r)|$ tends to be suppressed for $s_{\beta_3} \gtrsim 1$.

For the distance $r \gtrsim r_s$, both $-\phi'(r)$ and $\chi'(r)$ start to decrease as a function of r . When $s_{\beta_3} = 10^{-4}$, the distance r_V is of the order of $10 r_s$. Then, the solutions to $\phi'(r)$ and $\chi'(r)$ are given by Eq. (14.172) for $r_s < r \lesssim 10 r_s$ and by Eq. (14.170) for $r \gtrsim 10 r_s$. In fact, the behavior of the longitudinal mode changes from $\chi'(r) \propto r^{-1/2}$ to $\chi'(r) \propto r^{-2}$ around $r \approx 10 r_s$. For $s_{\beta_3} = 1$, the bottom panel of Fig. 14.4 shows that there is almost no intermediate regime given by the solution $\chi'(r) \propto r^{-1/2}$. Even if $s_{\beta_3} = \mathcal{O}(1)$, the quantity ξ in Eq. (14.168) soon gets larger than unity with the increase of r from r_s , such that the solutions for the distance $r > r_s$ are well approximated by Eq. (14.170) for $s_{\beta_3} \gtrsim 1$.

In Fig. 14.4, the temporal vector component $\phi(r)$ stays nearly constant both inside and outside the body. This is attributed to the fact that the r -dependent correction to $\phi(r)$ is at most of the order of $\phi_0 \Phi_*$, which is much smaller than ϕ_0 under the weak gravity approximation (14.148).

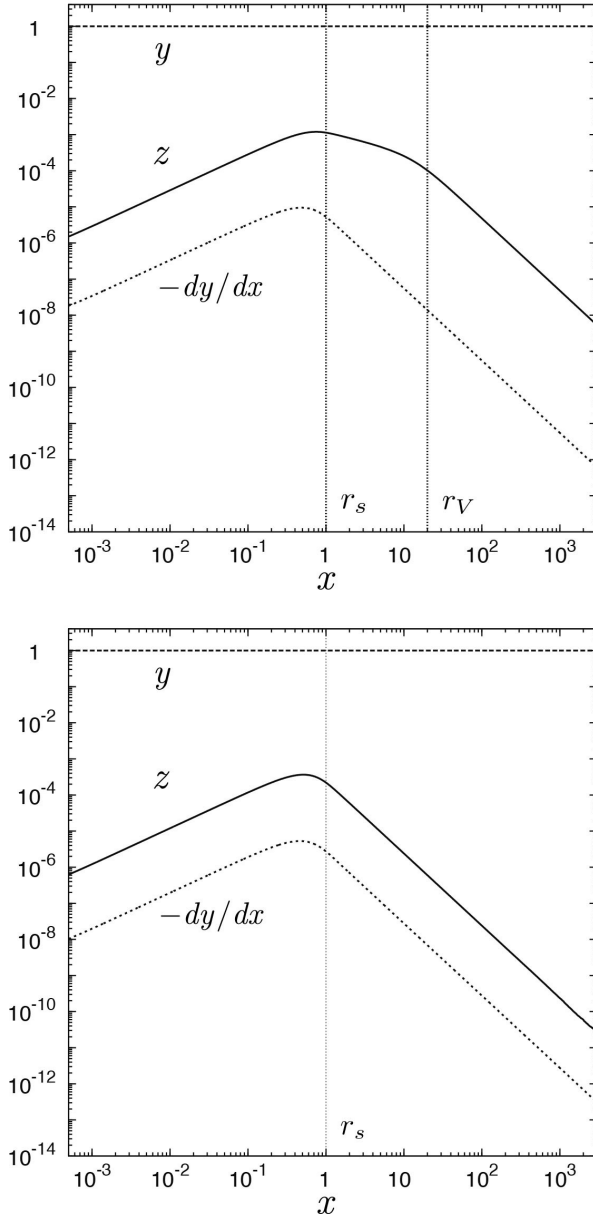


Fig. 14.4. Numerical solutions to $y = \phi/\phi_0$, $-dy/dx$, and $z = \chi'/\phi_0$ versus $x = r/r_s$ for the density profile (14.129) with $r_t = r_s/2$ with $\Phi_* = 10^{-4}$. The top and bottom panels correspond to $s_{\beta_3} = 10^{-4}$ and $s_{\beta_3} = 1$, respectively. We choose the boundary conditions of Ψ , Φ , y , and dy/dx to be consistent with Eqs. (14.146) and (14.161) at $x = 10^{-3}$. The vertical lines show the scales $r = r_s$ and $r_V = 20r_s$ (top panel) and the scale $r = r_s$ (bottom panel). The author thanks Ryotaro Kase for providing this figure.

14.3.1.3. *Corrections to gravitational potentials for $r > r_s$*

We derive corrections to leading-order gravitational potentials by using analytic field profiles in the regime $r > r_s$. First of all, the parameter s_{β_3} in Eq. (14.159) can be estimated as

$$\sqrt{s_{\beta_3}} \simeq 2.5 \times 10^{45} \beta_3 \frac{\phi_0}{M_{\text{pl}}} \sqrt{\frac{1 \text{ g/cm}^3}{\rho_0}}. \quad (14.173)$$

If we take the central density of the Sun ($\rho_0 \approx 100 \text{ g/cm}^3$), it follows that $\sqrt{s_{\beta_3}} \approx 10^{44} \beta_3 \phi_0 / M_{\text{pl}}$. Even if ϕ_0 is much smaller than the order of M_{pl} , it is natural to satisfy $s_{\beta_3} \gtrsim 1$ except for an extremely tiny coupling β_3 .

In the following, we shall focus on the coupling β_3 satisfying the condition $s_{\beta_3} \gtrsim 1$, in which case the field derivatives $\phi'(r)$ and $\chi'(r)$ at the distance $r > r_s$ are given by Eq. (14.170). Substituting the solutions (14.170) into Eqs. (14.142) and (14.143) and using the condition $\xi = s_{\beta_3} r^3 / r_s^3 \gg 1$, the gravitational potentials approximately obey the following differential equations outside the body:

$$\frac{2M_{\text{pl}}^2}{r} \Phi' + \frac{2M_{\text{pl}}^2}{r^2} \Phi = \Delta_{\Phi}, \quad (14.174)$$

$$\frac{2M_{\text{pl}}^2}{r} \Psi' - \frac{2M_{\text{pl}}^2}{r^2} \Phi = \Delta_{\Psi}, \quad (14.175)$$

where Δ_{Φ} and Δ_{Ψ} are correction terms given by

$$\Delta_{\Phi} \simeq \frac{5\Phi_*^2 \phi_0^2 r_s^2}{72r^4}, \quad \Delta_{\Psi} \simeq -\frac{\Phi_*^2 \phi_0^2 r_s^2}{72r^4}. \quad (14.176)$$

The integrated solutions to Eqs. (14.174) and (14.175) are expressed by the sum of the GR solutions (14.147) and those arising from the vector field, as

$$\Phi(r) \simeq \frac{\Phi_* r_s}{6r} \left[1 - \frac{5\Phi_*}{24} \left(\frac{\phi_0}{M_{\text{pl}}} \right)^2 \frac{r_s}{r} \right], \quad (14.177)$$

$$\Psi(r) \simeq -\frac{\Phi_* r_s}{6r} \left[1 - \frac{\Phi_*}{8} \left(\frac{\phi_0}{M_{\text{pl}}} \right)^2 \frac{r_s}{r} \right]. \quad (14.178)$$

Provided that the corrections $\Phi_*(\phi_0/M_{\text{pl}})^2(r_s/r)$ are smaller than the order of 1, the post-Newtonian parameter $\gamma = -\Phi/\Psi$ reduces to

$$\gamma \simeq 1 - \frac{\Phi_*}{12} \left(\frac{\phi_0}{M_{\text{pl}}} \right)^2 \frac{r_s}{r}. \quad (14.179)$$

The solar-system constraint (14.44) for the Sun ($\Phi_* \simeq 2.1 \times 10^{-6}$) translates to

$$\left(\frac{\phi_0}{M_{\text{pl}}} \right)^2 \frac{r_s}{r} < 1.3 \times 10^2. \quad (14.180)$$

For $r = \mathcal{O}(r_s)$, this bound is well satisfied if $\phi_0 \lesssim M_{\text{pl}}$. For larger r the deviation of γ from 1 decreases, so it is even easier to satisfy the constraint (14.44).

14.3.2. Quartic vector Galileons

Let us proceed to the model of quartic vector Galileons given by the functions

$$G_2(X) = m^2 X, \quad G_3(X) = 0, \quad G_4(X) = \frac{M_{\text{pl}}^2}{2} + \beta_4 X^2, \quad (14.181)$$

where β_4 is a constant having a dimension of $[\text{mass}]^{-2}$. In this case, Eqs. (14.139) and (14.140) reduce, respectively, to

$$\begin{aligned} \frac{1}{r^2} \frac{d}{dr} (r^2 \phi') - e^{2\Phi} m^2 \phi + 2\phi (\Psi'' + \Psi'^2 - \Psi' \Phi') + \left(3\phi' + \frac{4\phi}{r} \right) \Psi' - \phi' \Phi' \\ - \frac{2\beta_4 e^{-2\Phi} \phi}{r^2} [4r\chi' \chi'' + e^{2\Psi+2\Phi} \phi^2 (e^{2\Phi} - 1 + 2r\Phi') \\ - \chi'^2 \{ e^{2\Phi} - 3 + 2r(3\Phi' - 2\Psi') \}] = 0, \end{aligned} \quad (14.182)$$

$$\begin{aligned} \chi' \left\{ m^2 + \frac{2\beta_4}{r} \left[e^{2\Psi} \frac{\phi^2}{r} (1 - e^{-2\Phi}) + e^{2\Psi-2\Phi} (4\phi\phi' + 2\phi^2 \Psi') \right. \right. \\ \left. \left. - e^{-2\Phi} \frac{\chi'^2}{r} (1 - 3e^{-2\Phi} - 6r\Psi'e^{-2\Phi}) \right] \right\} = 0. \end{aligned} \quad (14.183)$$

Equation (14.183) admits the solution [49, 50]

$$\chi' = 0, \quad (14.184)$$

which corresponds to the perfect screening of the longitudinal mode. In this case, the modifications of gravity arise only by the temporal vector component $\phi(r)$. In the following, we estimate the corrections to gravitational potentials for the screened solution (14.184) of the longitudinal mode. In doing so, we employ the weak gravity approximation around a compact object (radius r_s and density ρ_0) and search for the profile of ϕ in the form (14.156). We also substitute the gravitational potentials (14.149) and (14.150) into Eq. (14.182) to derive the leading-order solution to $\phi(r)$.

For $r < r_s$, Eq. (14.182) reduces to

$$\frac{d}{dr} (r^2 \phi') + \phi_0 \Phi_* (1 - 2\beta_4 \phi_0^2) \frac{r^2}{r_s^2} \simeq 0. \quad (14.185)$$

Under the boundary condition $\phi'(0) = 0$, the integrated solution to Eq. (14.185) is given by

$$\phi'(r) \simeq - \frac{\phi_0 \Phi_* (1 - 2\beta_4 \phi_0^2)}{3r_s^2} r. \quad (14.186)$$

As long as the term $1 - 2\beta_4\phi_0^2$ is at most of the order of 1, the condition $|f(r)| \ll |\phi_0|$ is well satisfied in Eq. (14.156).

For $r > r_s$, we substitute Eq. (14.150) into Eq. (14.182) and pick up the first-order contributions of Φ and Ψ . This leads to

$$\frac{d}{dr} (r^2 \phi') \simeq 0, \quad (14.187)$$

whose integrated solution is given by $\phi'(r) = C/r^2$. The integration constant C is known by matching the interior and exterior solutions at $r = r_s$, so the solution outside the body reads

$$\phi'(r) \simeq -\frac{\phi_0 \Phi_* (1 - 2\beta_4 \phi_0^2)}{3r^2} r_s. \quad (14.188)$$

Substituting the exterior solution (14.188) into Eqs. (14.142) and (14.143) under the approximation of weak gravity, the gravitational potentials approximately obey Eqs. (14.174) and (14.175) with corrections

$$\Delta_\Phi \simeq -\frac{\phi_0^2 \Phi_*^2 r_s^2}{18r^4} (1 - 4\beta_4^2 \phi_0^4), \quad (14.189)$$

$$\Delta_\Psi \simeq \frac{\phi_0^2 \Phi_* r_s}{18r^4} [12\beta_4 \phi_0^2 r (1 - 4\beta_4 \phi_0^2) + \Phi_* r_s]. \quad (14.190)$$

These equations are integrated to give

$$\Phi(r) \simeq \frac{\Phi_* r_s}{6r} \left[1 + \frac{\phi_0^2 \Phi_* r_s}{6M_{\text{pl}}^2 r} (1 - 4\beta_4^2 \phi_0^4) \right], \quad (14.191)$$

$$\Psi(r) \simeq -\frac{\Phi_* r_s}{6r} \left[1 + \frac{2\beta_4 \phi_0^4}{M_{\text{pl}}^2} (1 - 4\beta_4 \phi_0^2) + \frac{\phi_0^2 \Phi_* r_s}{6M_{\text{pl}}^2 r} \right]. \quad (14.192)$$

As long as the correction terms in the square brackets of Eqs. (14.191) and (14.192) are smaller than the order of 1, the post-Newtonian parameter is approximately given by

$$\gamma \simeq 1 - \frac{2\beta_4 \phi_0^4}{M_{\text{pl}}^2} (1 - 4\beta_4 \phi_0^2). \quad (14.193)$$

From the solar-system constraint (14.44), it follows that

$$|\beta_4 \phi_0^4 (1 - 4\beta_4 \phi_0^2)| < 1 \times 10^{-5} M_{\text{pl}}^2. \quad (14.194)$$

If $|\beta_4| \phi_0^2 \ll 1$, then the condition (14.194) translates to $|\beta_4| \phi_0^4 < 1 \times 10^{-5} M_{\text{pl}}^2$. For ϕ_0 of the order of M_{pl} , the latter condition gives the bound $|\beta_4| \lesssim 10^{-5}/M_{\text{pl}}^2$. In this case, the condition $|\beta_4| \phi_0^2 \ll 1$ is automatically satisfied.

We have thus shown that derivative couplings arising for vector Galileons efficiently screen the propagation of the longitudinal mode. The cubic and quartic vector Galileons are consistent with local gravity constraints under mild bounds (14.180) and (14.194), respectively.

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Chapter 15

Effective Field Theory of Dark Energy

The effective field theory (EFT) of dark energy is a powerful framework to deal with low-energy scalar degrees of freedom in a systematic and unified way [1–6] (see also Refs. [7, 8] for the EFT of inflation). This approach is based on the expansion of a general four-dimensional action about the flat FLRW background in terms of the perturbations of three-dimensional geometric scalar quantities appearing in the $3 + 1$ Arnowitt–Deser–Misner (ADM) decomposition of spacetime [9]. Such geometric scalars consist of a lapse function N as well as traces and squares of an extrinsic curvature $K_{\mu\nu}$ and a three-dimensional intrinsic curvature ${}^{(3)}R_{\mu\nu}$ [10]. The Lagrangian can also depend on a scalar field ϕ and its kinetic energy X , but it is possible to absorb such dependence into the lapse by choosing a unitary gauge in which the field perturbation $\delta\phi$ vanishes.

The EFT formalism can accommodate a wide variety of modified gravity theories including Horndeski theories. In fact, the action of Horndeski theories can be expressed in terms of geometric scalar quantities mentioned above [10]. The EFT approach can encompass more general theories containing derivatives higher than second order. For example, Gleyzes–Langlois–Piazza–Vernizzi (GLPV) [11] performed a healthy extension of Horndeski theories without imposing two conditions Horndeski theories obey. Such generalizations can give rise to derivatives higher than second order, but the Hamiltonian analysis in the unitary gauge shows that the propagating scalar degrees of freedom remain to be one as in Horndeski theories [12–14]. Hence it is possible to go beyond the second-order domain of Horndeski theories by avoiding Ostrogradski instabilities.

The EFT approach can also encompass Lorentz-violating theories that contain spatial derivatives higher than second order. In Hořava–Lifshitz gravity [15], for example, an anisotropic scaling between time t and space x^i was introduced to suppress non-linear gravitational interactions in the ultraviolet regime. The existence of six spatial derivatives such as $\nabla_i {}^{(3)}R_{jk} \nabla^i {}^{(3)}R^{jk}$ allows the $z = 3$ scaling

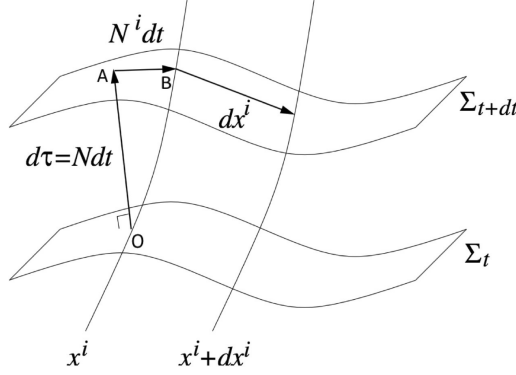


Fig. 15.1. Schematic view of the 3+1 decomposition of spacetime with a sequence of constant time hyper-surfaces Σ_t . The author thanks Takahiko Matsubara for providing the original figure.

characterized by the transformation $t \rightarrow c^3 t$ and $x^i \rightarrow c x^i$ (c is a constant), in which case the theory is power-counting renormalizable.

In this section, we review the EFT of dark energy in a very general framework including Horndeski theories, GLPV theories, and Hořava–Lifshitz gravity as specific cases. This unified scheme [16, 17] allows us to provide model-independent constraints on dark energy properties and to put constraints on individual models consistent with observations [18].

15.1. ADM decomposition of spacetime and EFT framework

We begin with foliating the four-dimensional spacetime into a sequence of constant time hyper-surfaces Σ_t labelled by t [9]. We express the distance between two hyper-surfaces Σ_t and Σ_{t+dt} (where dt is an infinitesimal time), as Ndt , where N is the lapse function (see Fig. 15.1). A unit covariant vector orthogonal to Σ_t is given by

$$n_\mu = -N\nabla_\mu t = (-N, 0, 0, 0). \quad (15.1)$$

The contravariant vector n^μ obeying the normalization $n_\mu n^\mu = -1$ corresponds to $n^\mu = (1/N, -N^i/N)$. The three-dimensional metric $q_{\mu\nu}$ induced on Σ_t is related to the four-dimensional metric $g_{\mu\nu}$ as [19]

$$q_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu, \quad (15.2)$$

which satisfies the relation $n^\mu q_{\mu\nu} = 0$. Multiplying Eq. (15.2) by $g^{\nu\lambda}$, we obtain $q_\mu^\lambda = \delta_\mu^\lambda + n_\mu n^\lambda$. Multiplying this equation by $g^{\mu\rho}$ gives $q^{\lambda\rho} = g^{\lambda\rho} + n^\lambda n^\rho$. On using the relation $g_{\mu\nu} g^{\nu\rho} = \delta_\mu^\rho$, it follows that

$$q_\mu^\rho = q_{\mu\nu} q^{\nu\rho} = \delta_\mu^\rho + n_\mu n^\rho. \quad (15.3)$$

In Fig. 15.1, we show the vector field n^μ orthogonal to Σ_t on a spacetime point O (with the spatial coordinate x^i), which intersects with the point A on Σ_{t+dt} . The

point B whose coordinate corresponds to x^i on Σ_{t+dt} is generally different from the point A. This difference is quantified by $N^i dt$, where N^i is called a shift vector. On using the lapse and shift functions as well as the three-dimensional metric q_{ij} , the four-dimensional line element can be expressed in the form

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu = -N^2 dt^2 + q_{ij} (dx^i + N^i dt)(dx^j + N^j dt). \quad (15.4)$$

The non-vanishing components of $g_{\mu\nu}$ are given, respectively, by

$$g_{00} = -N^2 + N^i N_i, \quad g_{0i} = g_{i0} = N_i, \quad g_{ij} = h_{ij}. \quad (15.5)$$

The inverse metrics are

$$g^{00} = -\frac{1}{N^2}, \quad g^{0i} = g^{i0} = \frac{N^i}{N^2}, \quad g^{ij} = h^{ij} - \frac{N^i N^j}{N^2}. \quad (15.6)$$

From a vector field ω^μ in the four-dimensional spacetime, we can construct the three-dimensional vector field $\tilde{\omega}^\nu$ living on Σ_t , as

$$\tilde{\omega}^\nu \equiv q_\mu^\nu \omega^\mu, \quad (15.7)$$

where $q_\mu^\nu = q_{\mu\lambda} g^{\nu\lambda}$. Indeed, the vector field $\tilde{\omega}^\nu$ obeys the orthogonal relation $n_\nu \tilde{\omega}^\nu = n_\nu q_\mu^\nu \omega^\mu = 0$. Thus, the metric $q_{\mu\nu}$ works as a projection operator on Σ_t .

We define the covariant derivative D_j for the vector field $\tilde{\omega}^i$ as

$$D_j \tilde{\omega}^i = q_a^i q_j^b \nabla_b \tilde{\omega}^a. \quad (15.8)$$

Acting the operator D_k on the metric q_{ij} , it follows that

$$D_k q_{ij} = q_k^a q_i^b q_j^c \nabla_a q_{bc} = q_k^a q_i^b q_j^c \nabla_a (g_{bc} + n_b n_c) = 0, \quad (15.9)$$

where we used the property $\nabla_a g_{bc} = 0$. Hence the standard property of the four-dimensional covariant derivative also holds on Σ_t for the operator D_j defined by Eq. (15.8). From Eq. (15.9), we can express the three-dimensional Christoffel symbol ${}^{(3)}\Gamma_{jk}^i$ as that in the four-dimensional case, i.e.,

$${}^{(3)}\Gamma_{jk}^i = \frac{1}{2} q^{il} (q_{lj,k} + q_{lk,j} - q_{jk,l}). \quad (15.10)$$

The covariant derivative $\nabla_\mu n_\nu$ with respect to $g_{\mu\nu}$ corresponds to the change induced by the parallel transport of n_ν in four dimensions. To quantify the change

induced by the parallel transport of n_ν on Σ_t , we define the extrinsic curvature

$$K_{ij} \equiv q_i^\alpha q_j^\beta \nabla_\alpha n_\beta = \frac{1}{2} q_i^\alpha q_j^\beta (\nabla_\alpha n_\beta + \nabla_\beta n_\alpha). \quad (15.11)$$

On using the property $n^\beta \nabla_\alpha n_\beta = 0$, we have $q_i^\alpha q_j^\beta \nabla_\alpha n_\beta = (g_i^\alpha + n_i n^\alpha) g_j^\beta \nabla_\alpha n_\beta$, so the extrinsic curvature can be expressed as

$$K_{ij} = \nabla_i n_j + n_i a_j, \quad (15.12)$$

where a_j is called the acceleration vector defined by

$$a_j \equiv n^\alpha \nabla_\alpha n_j. \quad (15.13)$$

Substituting $n_j = -N \nabla_j t$ into Eq. (15.13) and using the relations $\nabla_\alpha \nabla_j t = \nabla_j \nabla_\alpha t$ and $q_j^\alpha = \delta_j^\alpha + n^\alpha n_j$, we obtain

$$\begin{aligned} a_j &= -n^\alpha \nabla_\alpha N \nabla_j t - n^\alpha N \nabla_j \nabla_\alpha t \\ &= n^\alpha n_j N^{-1} \nabla_\alpha N + n^\alpha N \nabla_j (N^{-1} n_\alpha) \\ &= (n^\alpha n_j + \delta_j^\alpha) \nabla_\alpha \ln N \\ &= D_j \ln N. \end{aligned} \quad (15.14)$$

If the lapse N depends on t alone, the acceleration vector vanishes.

Since the extrinsic curvature is a symmetric tensor, we have $K_{ij} = (K_{ij} + K_{ji})/2$. Then, from Eq. (15.12), it follows that

$$\begin{aligned} K_{ij} &= \frac{1}{2} [\nabla_i n_j + \nabla_j n_i + n^\alpha \nabla_\alpha (n_i n_j)] \\ &= \frac{1}{2} (q_{j\mu} \nabla_i n^\mu + q_{i\nu} \nabla_j n^\nu + n^\alpha \nabla_\alpha q_{ij}) \\ &= \frac{1}{2} (q_{j\mu} \partial_i n^\mu + q_{i\nu} \partial_j n^\nu + n^\alpha \partial_\alpha q_{ij}), \end{aligned} \quad (15.15)$$

where in the last line we used the relations $\nabla_i n^\mu = \partial_i n^\mu + \Gamma_{\alpha i}^\mu n^\alpha$ and $\nabla_\alpha q_{ij} = \partial_\alpha q_{ij} - \Gamma_{i\alpha}^\beta q_{\beta j} - \Gamma_{j\alpha}^\beta q_{i\beta}$. In terms of the three-dimensional covariant derivative $D_i N_j = \partial_i N_j - {}^{(3)}\Gamma_{ij}^k N_k$ of the shift vector N_j , where ${}^{(3)}\Gamma_{ij}^k$ is the Christoffel symbol associated with respect to h_{ij} , we can write Eq. (15.15) as

$$K_{ij} = \frac{1}{2N} (\partial_t h_{ij} - D_i N_j - D_j N_i). \quad (15.16)$$

Hence the extrinsic curvature can be regarded as a “kinetic term” containing a time derivative of h_{ij} .

The internal geometry of Σ_t can be quantified in terms of the three-dimensional Ricci tensor

$$\mathcal{R}_{ij} \equiv {}^{(3)}R_{ij}, \quad (15.17)$$

which is called the intrinsic curvature. This three-dimensional quantity contains spatial derivatives of h_{ij} , so the intrinsic curvature is a quantity associated with a “potential term”.

In GR, the gravitational Lagrangian is given by the four-dimensional Ricci scalar R , so we first express R in terms of ADM geometric quantities introduced above. As an extension of the four-dimensional Riemann tensor satisfying Eq. (3.47), the three-dimensional Riemann tensor $\mathcal{R}_{ijk}{}^l \equiv {}^{(3)}R_{ijk}{}^l$ on Σ_t can be defined according to the relation

$$(D_i D_j - D_j D_i) \tilde{\omega}_k = \mathcal{R}_{ijk}{}^l \tilde{\omega}_l, \quad (15.18)$$

where the three-dimensional vector field $\tilde{\omega}_k$ obeys $n^k \tilde{\omega}_k = 0$. From the definition of the three-dimensional covariant derivative, it follows that

$$\begin{aligned} D_i D_j \tilde{\omega}_k &= q_i^a q_j^b q_k^c \nabla_a (q_b^l q_c^m \nabla_l \tilde{\omega}_m) \\ &= q_i^a q_j^b q_k^c \nabla_a \nabla_b \tilde{\omega}_c + q_i^a q_j^b q_k^m (\nabla_a q_b^l) (\nabla_l \tilde{\omega}_m) + q_i^a q_j^l q_k^c (\nabla_a q_c^m) (\nabla_l \tilde{\omega}_m). \end{aligned} \quad (15.19)$$

The four-dimensional covariant derivative of q_a^b reads

$$\begin{aligned} \nabla_c q_a^b &= \nabla_c (n_a n^b) = n_a \nabla_c n^b + n^b \nabla_c n_a \\ &= n_a (K_c^b - n_c D^b \ln N) + n^b (K_{ac} - n_c D_a \ln N). \end{aligned} \quad (15.20)$$

Multiplication $\nabla_c q_a^b$ by $q_i^c q_j^a$, it follows that

$$q_i^c q_j^a \nabla_c q_a^b = n^b K_{ij}. \quad (15.21)$$

On using the relation $n^m \tilde{\omega}_m = 0$, we have

$$q_j^l n^m \nabla_l \tilde{\omega}_m = -q_j^l \tilde{\omega}_m \nabla_l n^m = -\tilde{\omega}_m K_j^m. \quad (15.22)$$

Then, Eq. (15.19) reduces to

$$D_i D_j \tilde{\omega}_k = q_i^a q_j^b q_k^c \nabla_a \nabla_b \tilde{\omega}_c + (n^a \nabla_a \tilde{\omega}_m) q_k^m K_{ij} - K_{ik} K_j^m \tilde{\omega}_m, \quad (15.23)$$

so the left hand side of Eq. (15.18) yields

$$(D_i D_j - D_j D_i) \tilde{\omega}_k = q_i^a q_j^b q_k^c R_{abc}{}^l \tilde{\omega}_l - K_j^l K_{ik} \tilde{\omega}_l + K_i^l K_{jk} \tilde{\omega}_l. \quad (15.24)$$

Comparing this with the right hand side of Eq. (15.18), we obtain the following Gauss–Codacci equation

$$\mathcal{R}_{ijkl} = q_i^a q_j^b q_k^c q_l^d R_{abcd} + K_{il} K_{jk} - K_{ik} K_{jl}. \quad (15.25)$$

Multiplying Eq. (15.25) by $q^{ik} = g^{ik} + n^i n^k$, the three-dimensional Ricci tensor $\mathcal{R}_{jl}$ can be expressed as

$$\mathcal{R}_{jl} = q_j^b q_l^d (R_{bd} + R_{abcd} n^a n^c) + K_{jk} K_l^k - K K_{jl}, \quad (15.26)$$

where

$$K \equiv q^{ij} K_{ij}. \quad (15.27)$$

The three-dimensional Ricci scalar is defined by

$$\mathcal{R} \equiv q^{jl} \mathcal{R}_{jl}. \quad (15.28)$$

On using Eq. (15.26) and the relation $R_{abcd} n^a n^b n^c n^d = 0$ (which follows from the anti-symmetric property $R_{abcd} = -R_{bacd}$), it follows that

$$\mathcal{R} = R + 2R_{ab} n^a n^b + \mathcal{S} - K^2, \quad (15.29)$$

where

$$\mathcal{S} \equiv K_{ij} K^{ij}. \quad (15.30)$$

Since the Einstein tensor $G_{ab} = R_{ab} - g_{ab} R/2$ obeys the relation $n^a n^b G_{ab} = n^a n^b R_{ab} + R/2$, we can express the relation (15.29) in the simple form

$$\mathcal{R} = 2n^a n^b G_{ab} + \mathcal{S} - K^2. \quad (15.31)$$

The quantity $R_{ab} n^a n^b$ in Eq. (15.29) is given by

$$\begin{aligned} R_{ab} n^a n^b &= R_{acb}^c n^a n^b \\ &= n^a (\nabla^c \nabla_a - \nabla_a \nabla^c) n_c \\ &= \nabla^c (n_a \nabla^a n_c - n_c \nabla^a n_a) - \nabla^c n_a \nabla^a n_c + \nabla^c n_c \nabla^a n_a \\ &= \nabla^\mu (a_\mu - K n_\mu) - \mathcal{S} + K^2, \end{aligned} \quad (15.32)$$

where, in the last line, we used the acceleration vector $a_\mu = n_a \nabla^a n_\mu$ and the trace $K = \nabla^a n_a$ of the extrinsic curvature. Substituting Eq. (15.32) into Eq. (15.29), the four-dimensional Ricci scalar can be expressed as

$$R = \mathcal{R} - K^2 + \mathcal{S} + 2\nabla^\mu (K n_\mu - a_\mu). \quad (15.33)$$

On using the relation (3.93), the integral $\int d^4x \sqrt{-g} \nabla^\mu (K n_\mu - a_\mu)$ reduces to a boundary term irrelevant to the dynamical equations of motion. Hence the Einstein–Hilbert action $S_{\text{EH}} = (M_{\text{pl}}^2/2) \int d^4x \sqrt{-g} R$ reads

$$S_{\text{EH}} = \frac{M_{\text{pl}}^2}{2} \int dt d^3x N \sqrt{q} (\mathcal{R} - K^2 + \mathcal{S}), \quad (15.34)$$

where q is the determinant of q_{ij} . The action (15.34) consists of two kinetic terms $\mathcal{S}, K$ and the potential term $\mathcal{R}$.

Since we would like to construct the EFT of dark energy with one scalar field ϕ coupled to gravity, we consider possible geometric scalar combinations in the following. First of all, the three-dimensional Riemann tensor ${}^{(3)}R_{\mu\nu\rho\sigma}$ can be expressed in terms of the Ricci tensor and Ricci scalar in three dimensions, so it is not necessary to take into account scalar quantities constructed from ${}^{(3)}R_{\mu\nu\rho\sigma}$. Besides the ADM variables $N, K, \mathcal{S}, \mathcal{R}$ appearing in the action (15.34), we can consider the combination

$$\mathcal{U} \equiv \mathcal{R}_{\mu\nu} K^{\mu\nu}. \quad (15.35)$$

As we will see in Sec. 15.2.1, the action of Horndeski theories can be expressed in terms of $N, K, \mathcal{S}, \mathcal{R}, \mathcal{U}$ by choosing the so-called unitary gauge in which the field perturbation $\delta\phi$ vanishes.

Horndeski theories are Lorentz-invariant theories whose equations of motion remain of second order in both time and spatial derivatives. In Lorentz-violating theories like Hořava–Lifshitz gravity (which we will discuss in Sec. 15.2.2) there are spatial derivatives higher than second order. Now, we allow for the existence of scalar quantities up to sixth-order spatial derivatives to encompass Hořava–Lifshitz gravity in our general EFT scheme. Then, we can consider the following combinations

$$\mathcal{Z} \equiv \mathcal{R}_{ij} \mathcal{R}^{ij}, \quad \mathcal{Z}_1 \equiv D_i \mathcal{R} D^i \mathcal{R}, \quad \mathcal{Z}_2 \equiv D_i \mathcal{R}_{jk} D^i \mathcal{R}^{jk}, \quad (15.36)$$

and $\mathcal{Z}_3 \equiv \mathcal{R}_i^j \mathcal{R}_j^k \mathcal{R}_k^i$, $\mathcal{Z}_4 \equiv \mathcal{R} \mathcal{R}_i^j \mathcal{R}_j^i$. The terms $\mathcal{Z}_3$ and $\mathcal{Z}_4$ do not affect the dynamics of linear cosmological perturbations on the flat FLRW background, so we do not include such contributions.

In the original Hořava–Lifshitz gravity [15] the lapse N depends on the time t alone (which is called the projectability condition), reflecting the fact that the space-time foliation is preserved by the space-independent reparametrization $t \rightarrow t'(t)$. In this case the acceleration vector $a_j = D_j \ln N$ vanishes, so the extrinsic curvature reduces to $K_{ij} = \nabla_i n_j$. The original Hořava–Lifshitz theory, which is plagued by a strong-coupling problem [20, 21], can be healthily extended in such a way that the lapse depends on the spatial coordinate x^i ($i = 1, 2, 3$) as well as time t [22]. In this non-projectable version of the Hořava–Lifshitz gravity, the acceleration vector does not vanish, so we can take into account scalar combinations constructed from a_i , as

$$\alpha_1 \equiv a_i a^i, \quad \alpha_2 \equiv a_i \Delta a^i, \quad \alpha_3 \equiv \mathcal{R} D_i a^i, \quad \alpha_4 \equiv a_i \Delta^2 a^i, \quad \alpha_5 \equiv \Delta \mathcal{R} D_i a^i, \quad (15.37)$$

where $\Delta \equiv D_i D^i$. There are also other contributions like $(a_i a^i)^2$ and $a_i a_j \mathcal{R}^{ij}$, but we do not take into account such terms since they are irrelevant to the dynamics of linear scalar perturbations on the flat FLRW background [23].

The action of modified gravitational theories containing the aforementioned scalar quantities is given by [16, 17]

$$S = \int d^4x \sqrt{-g} \mathcal{L}(N, K, \mathcal{S}, \mathcal{R}, \mathcal{U}, \mathcal{Z}, \mathcal{Z}_1, \mathcal{Z}_2, \alpha_1, \dots, \alpha_5; t), \quad (15.38)$$

where the time t is included for the reason explained later in Sec. 15.2.1. The equations of motion for linear cosmological perturbations follow by expanding the action (15.38) up to second order in perturbations. Before doing so, we review theories that can be encompassed in the above general framework.

15.2. Concrete theories in terms of the ADM language

In this section, we study how the Lagrangians L of concrete modified gravity theories depend on geometric scalar quantities appearing in the ADM formalism. We will focus on two classes of theories: (i) Horndeski theories and generalizations, and (ii) Hořava–Lifshitz gravity.

15.2.1. Horndeski theories and generalizations

The action of Horndeski theories is given by Eq. (12.1) with the Lagrangian densities (12.2)–(12.5). In the following, we choose the unitary gauge

$$\phi = \phi(t), \quad (15.39)$$

under which the field perturbation $\delta\phi(t, x^i)$ vanishes. For this gauge choice, the field kinetic energy $X = -g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi/2$ reads

$$X = \frac{\dot{\phi}^2(t)}{2N^2}. \quad (15.40)$$

Hence the ϕ and X dependence in the functions $G_{2,3,4,5}$ can be interpreted as the N and t dependence in the action (15.38).

In the unitary gauge, the constant- ϕ hyper-surface coincides with Σ_t , so the unit vector orthogonal to those hyper-surfaces is given by [10]

$$n_\mu = -\gamma\nabla_\mu\phi, \quad \gamma = \frac{1}{\sqrt{2X}}. \quad (15.41)$$

Using the relation (15.12) and taking the covariant derivative of Eq. (15.41), it follows that

$$\nabla_\mu\nabla_\nu\phi = -\frac{1}{\gamma}(K_{\mu\nu} - n_\mu a_\nu - n_\nu a_\mu) - \gamma^2 n_\mu n_\nu \nabla^\lambda\phi\nabla_\lambda X. \quad (15.42)$$

Multiplying Eq. (15.42) by $g^{\mu\nu}$, we obtain

$$\square\phi = -\frac{K}{\gamma} + \frac{\nabla^\lambda\phi\nabla_\lambda X}{2X}, \quad (15.43)$$

so the cubic-order Lagrangian density (12.3) can be expressed as $\mathcal{L}_3 = G_3[K/\gamma - \nabla^\lambda\phi\nabla_\lambda X/(2X)]$. We introduce an auxiliary function $F_3(\phi, X)$ satisfying

$$G_3 = F_3 + 2XF_{3,X}. \quad (15.44)$$

The contribution $F_3 \square \phi$ is equivalent to $-(F_{3,\phi} \nabla_\lambda \phi + F_{3,X} \nabla_\lambda X) \nabla^\lambda \phi$ up to a boundary term, whose second term is cancelled by one of the terms arising from $2X F_{3,X} \square \phi$. Then, the cubic-order Lagrangian density can be expressed as

$$\mathcal{L}_3 = (2X)^{3/2} F_{3,X} K - 2X F_{3,\phi}. \quad (15.45)$$

Since F_3 depends on $\phi(t)$ and $X(t, N) = \dot{\phi}^2(t)/(2N^2)$, $\mathcal{L}_3$ is a function of N , K , and t . Although $\mathcal{L}_3$ contains an auxiliary function F_3 , the equations of motion following from Eq. (15.45) can be written in terms of G_3 and its derivatives with respect to ϕ and X [10].

The next step is to substitute Eqs. (15.42) and (15.43) into the quartic Lagrangian density (12.4) on account of the relations $\gamma^{-2} = 2X$ and $a_\mu = -q_\mu^\nu \nabla_\nu X/(2X)$. This leads to

$$\begin{aligned} \mathcal{L}_4 &= G_4 R + G_{4,X} \left[\left(-\frac{K}{\gamma} + \gamma^2 \nabla^\lambda \phi \nabla_\lambda X \right)^2 - \frac{1}{\gamma^2} (\mathcal{S} - 2a_\mu a^\mu) - \gamma^4 (\nabla^\lambda \phi \nabla_\lambda X)^2 \right] \\ &= G_4 R + 2X G_{4,X} (K^2 - \mathcal{S}) + 2G_{4,X} (K n^\mu - a^\mu) \nabla_\mu X. \end{aligned} \quad (15.46)$$

On using Eq. (15.33) together with the relations $G_{4,X} \nabla_\mu X = \nabla_\mu G_4 + \gamma^{-1} G_{4,\phi} n_\mu$ and $n_\mu a^\mu = 0$, the Lagrangian density (15.46) reduces

$$\mathcal{L}_4 = G_4 \mathcal{R} + (2X G_{4,X} - G_4) (K^2 - \mathcal{S}) - 2\sqrt{2X} G_{4,\phi} K, \quad (15.47)$$

up to boundary terms. Hence the quartic Horndeski Lagrangian density depends on N , K , $\mathcal{S}$, $\mathcal{R}$, and t .

To express the quintic Lagrangian density (12.5) in terms of the ADM scalar quantities, we first integrate the term $G_5 G_{\mu\nu} \nabla^\mu \nabla^\nu \phi$ by parts, as

$$G_5 G_{\mu\nu} \nabla^\mu \nabla^\nu \phi = -G_{5,X} \nabla^\mu X \nabla^\nu \phi G_{\mu\nu} - \gamma^{-2} G_{5,\phi} G_{\mu\nu} n^\mu n^\nu. \quad (15.48)$$

As in the case of the cubic Lagrangian, we introduce an auxiliary function $F_5(\phi, X)$, as

$$G_{5,X} \equiv \frac{F_5}{2X} + F_{5,X}. \quad (15.49)$$

Then, the term $G_{5,X} \nabla^\mu X$ can be expressed in the form

$$G_{5,X} \nabla^\mu X = \gamma \nabla^\mu (\gamma^{-1} F_5) + \gamma^{-1} F_{5,\phi} n^\mu. \quad (15.50)$$

Employing this relation for Eq. (15.48) and integrating it by parts, we obtain

$$G_5 G_{\mu\nu} \nabla^\mu \nabla^\nu \phi = F_5 G_{\mu\nu} \nabla^\mu \nabla^\nu \phi + \gamma F_{5,X} G_{\mu\nu} n^\mu n^\nu + \gamma^{-2} (F_{5,\phi} - G_{5,\phi}) G_{\mu\nu} n^\mu n^\nu. \quad (15.51)$$

The product $K^{\mu\nu}G_{\mu\nu}$ arises after substituting Eq. (15.42) with upper indices into Eq. (15.51). To compute this product, we multiply Eq. (15.26) by q^{jl} . This leads to the following relation:

$$K^{\mu\nu}G_{\mu\nu} = K^{\mu\nu}\mathcal{R}_{\mu\nu} - \frac{1}{2}KR + K\mathcal{S} - K_{ij}K^{il}K^j{}_l - K^{\mu\nu}R_{\rho\mu\lambda\nu}n^\rho n^\lambda, \quad (15.52)$$

which is used for the computation of Eq. (15.51).

On using Eqs. (15.42) and (15.43), the rest of terms in Eq. (12.5) can be expressed as

$$\begin{aligned} & -\frac{1}{6}G_{5,X} [(\Box\phi)^3 - 3(\Box\phi)(\nabla_\mu\nabla_\nu\phi)(\nabla^\mu\nabla^\nu\phi) + 2(\nabla^\mu\nabla_\nu\phi)(\nabla^\nu\nabla_\lambda\phi)(\nabla^\lambda\nabla_\mu\phi)] \\ & = \frac{1}{6}G_{5,X}\gamma^{-3}K_3 - \frac{1}{2}G_{5,X}\mathcal{Q}, \end{aligned} \quad (15.53)$$

where

$$K_3 \equiv K^3 - 3KK_{ij}K^{ij} + 2K_{ij}K^{il}K^j{}_l, \quad (15.54)$$

$$\mathcal{Q} \equiv \nabla^\mu\phi\nabla_\mu X (K^2 - \mathcal{S}) - 2\gamma^{-3}(Ka_\mu a^\mu - K_{\mu\nu}a^\mu a^\nu). \quad (15.55)$$

On using the auxiliary function F_5 with the integration by parts, the second term on the right hand side of Eq. (15.53) can be expressed as

$$\begin{aligned} -\frac{1}{2}G_{5,X}\mathcal{Q} &= -F_5\gamma^{-1}\left(\frac{1}{2}K_3 - Kn^\mu n^\nu R_{\mu\nu} + K^{\mu\nu}n^\rho n^\sigma R_{\mu\rho\nu\sigma} + a^\mu n^\nu R_{\mu\nu}\right) \\ &\quad - \frac{\gamma^{-2}}{2}F_{5,\phi}(K^2 - \mathcal{S}). \end{aligned} \quad (15.56)$$

Now, we take the sum of Eqs. (15.51) and (15.53) on account of Eqs. (15.42), (15.52) and (15.56). We also employ the relation $G_{\mu\nu}n^\mu n^\nu = (\mathcal{R} + K^2 - \mathcal{S})/2$ following from Eq. (15.31). Then, the resulting quintic Lagrangian density reads

$$\begin{aligned} \mathcal{L}_5 &= X(F_{5,\phi} - G_{5,\phi})\mathcal{R} - XG_{5,\phi}(K^2 - \mathcal{S}) + \frac{1}{6}(2X)^{3/2}G_{5,X}K_3 \\ &\quad - \sqrt{2X}F_5\left(\mathcal{U} - \frac{1}{2}K\mathcal{R}\right), \end{aligned} \quad (15.57)$$

which depends on $N, K, \mathcal{S}, \mathcal{R}, \mathcal{U}, K_3$, and t . On the flat FLRW background with the Hubble expansion rate H , the term K_3 can be expanded up to quadratic order in perturbations as

$$K_3 = 3H(2H^2 - 2KH + K^2 - \mathcal{S}) + \mathcal{O}(3), \quad (15.58)$$

which depends on K and $\mathcal{S}$ only. Hence, as long as linear cosmological perturbations are concerned, the EFT approach based on the action (15.38) can encompass the quintic-order Horndeski theory.

From Eqs. (12.2), (15.45), (15.47) and (15.57), the total action of Horndeski theories can be written as $S = \int dt d^3x N \sqrt{q} \mathcal{L}$ with the Lagrangian density [10]

$$\begin{aligned} \mathcal{L} = & A_2(N, t) + A_3(N, t)K + A_4(N, t)(K^2 - \mathcal{S}) + B_4(N, t)\mathcal{R} \\ & + A_5(N, t)K_3 + B_5(N, t) \left(\mathcal{U} - \frac{1}{2}K\mathcal{R} \right), \end{aligned} \quad (15.59)$$

where

$$\begin{aligned} A_2 &= G_2 - 2X F_{3,\phi}, & A_3 &= (2X)^{3/2} F_{3,X} - 2\sqrt{2X} G_{4,\phi}, \\ A_4 &= 2X G_{4,X} - G_4 - X G_{5,\phi}, & B_4 &= G_4 + X(F_{5,\phi} - G_{5,\phi}), \\ A_5 &= \frac{1}{6}(2X)^{3/2} G_{5,X}, & B_5 &= -\sqrt{2X} F_5. \end{aligned} \quad (15.60)$$

Among the coefficients A_4, B_4 and A_5, B_5 , there are two particular relations

$$A_4 = 2X B_{4,X} - B_4, \quad A_5 = -\frac{1}{3}X B_{5,X}, \quad (15.61)$$

under which the number of free functions reduces from six to four.

GLPV generalized Horndeski theories in such a way that the coefficients A_4, B_4, A_5, B_5 do not necessarily satisfy the two relations (15.61) [11]. This generally gives rise to derivatives higher than second order, but the Hamiltonian analysis in the unitary gauge shows that the number of scalar propagating degrees of freedom remains one at the fully non-linear level [12–14]. Hence it is possible to construct healthy theories beyond Horndeski without Ostrogradski instabilities. As in Horndeski theories, the Lagrangian density of GLPV theories contains the dependence of $N, K, \mathcal{S}, \mathcal{R}, \mathcal{U}$, and t . In terms of the four-dimensional covariant Language, the new terms arising from the breaking of two conditions (15.61) correspond to the detunings of coefficients between G_4 and $G_{4,X}$ as well as between G_5 and $G_{5,X}$. As in the construction of the Galileon Lagrangians given by Eq. (11.127), the two new Lagrangian densities in GLPV theories can be expressed as

$$\begin{aligned} \mathcal{L}_4^{\text{GLPV}} &= F_4(\phi, X) \epsilon^{\mu\nu\rho\sigma} \epsilon_{\mu'\nu'\rho'\sigma'} \nabla^{\mu'} \phi \nabla_\mu \phi \nabla^{\nu'} \nabla_\nu \phi \nabla^{\rho'} \nabla_\rho \phi, \\ \mathcal{L}_5^{\text{GLPV}} &= F_5(\phi, X) \epsilon^{\mu\nu\rho\sigma} \epsilon_{\mu'\nu'\rho'\sigma'} \nabla^{\mu'} \phi \nabla_\mu \phi \nabla^{\nu'} \nabla_\nu \phi \nabla^{\rho'} \nabla_\rho \phi \nabla^{\sigma'} \nabla_\sigma \phi, \end{aligned} \quad (15.62)$$

$$(15.63)$$

where F_4 and F_5 are functions of ϕ and X .

15.2.2. Hořava–Lifshitz gravity

Hořava–Lifshitz gravity [15] is an attempt for constructing a power-counting renormalized theory of gravity in the ultra-violet regime. In Hořava–Lifshitz gravity, the Lorentz invariance is broken to suppress non-linear graviton interactions higher than sixth order. While this theory is not directly related to the infra-red modification

of gravity, we incorporate it as an example of containing spatial derivatives higher than second order.

To understand the power-counting renormalizability of Hořava–Lifshitz gravity, let us begin with the following anisotropic scaling in time (t) and space (x) on the Minkowski spacetime:

$$t \rightarrow c^z t, \quad x \rightarrow cx, \quad (15.64)$$

where c is an arbitrary number, and z is a power-law index dubbed dynamical critical exponent. We consider a canonical scalar field φ transforming as $\varphi \rightarrow c^s \varphi$ under the scaling (15.64). The kinetic action of a canonical scalar field φ transforms as

$$\int dt d^3x \frac{1}{2} \dot{\varphi}^2 \rightarrow c^{3-z+2s} \int dt d^3x \frac{1}{2} \dot{\varphi}^2, \quad (15.65)$$

which is invariant under the choice

$$s = \frac{z-3}{2}. \quad (15.66)$$

If $z = 3$, then the scalar field is unchanged under the anisotropic scaling (15.64).

Under (15.64), the n th order interaction term φ^n transforms as

$$\int dt d^3x \varphi^n \rightarrow c^{z+3+ns} \int dt d^3x \varphi^n \propto E^{-(z+3+ns)/z} \int dt d^3x \varphi^n, \quad (15.67)$$

where we used the fact that the energy E scales as $E \rightarrow c^{-z} E$. For $z = 3$ with Eq. (15.66), the exponent $-(z+3+ns)/z$ is -2 for any value of n , so non-linear interactions are power-counting renormalizable [24]. This power-counting renormalizability also persists under the anisotropic scaling with $z > 3$.

The example of a scalar-field action invariant under the $z = 3$ scaling is given by

$$S_{\text{UV}} = \int dt d^3x \left(\frac{1}{2} \dot{\varphi}^2 + \frac{\varphi \Delta^3 \varphi}{M^4} \right), \quad (15.68)$$

where $\Delta = \partial_i \partial^i$, and M is a constant having a dimension of mass. Taking into account the Lagrangians $\varphi \Delta^2 \varphi$ and $\varphi \Delta \varphi$ invariant under the $z = 2$ and $z = 1$ scalings, respectively, the total action reads

$$S = \int dt d^3x \left(\frac{1}{2} \dot{\varphi}^2 + \frac{\varphi \Delta^3 \varphi}{M^4} + \frac{c_1 \varphi \Delta^2 \varphi}{M^2} + c_s^2 \varphi \Delta \varphi \right), \quad (15.69)$$

where c_1 is a constant, and c_s is the sound speed of ϕ . In the ultra-violet (small-scale) limit, the second term on the right hand side of Eq. (15.69) dominates over the third and fourth terms, so the action (15.69) reduces to Eq. (15.68). In this regime, non-linear field interactions φ^n are suppressed due to the $z = 3$ scaling. In the infra-red limit the second and third terms of Eq. (15.69) are suppressed relative to the fourth one, so the corresponding infra-red action $S_{\text{IR}} = \int dt d^3x (\dot{\varphi}^2/2 + c_s^2 \varphi \Delta \varphi)$ is invariant under the $z = 1$ scaling.

The above idea of anisotropic scaling can be applied to the construction of a power-counting renormalizable gravitational theory. Since the time has a privileged role in the anisotropic scaling, the theory should respect the symmetry under time reparametrization and time-dependent spatial diffeomorphism given by

$$t \rightarrow \tilde{t}(t), \quad x^i \rightarrow \tilde{x}^i(t, x^i), \quad (i = 1, 2, 3), \quad (15.70)$$

which breaks the Lorentz symmetry in four-dimensional spacetime. Here, the time reparametrization does not depend on spatial coordinates. Since the spacetime foliation is preserved by the transformation (15.70), this mapping is called the foliation preserving diffeomorphism.

Under the infinitesimal transformations $t \rightarrow t + f(t)$ and $x^i \rightarrow x^i + \xi^i(t, x^i)$, the lapse N , the shift N_i , and the three-dimensional metric q_{ij} in Eq. (15.4) transform as

$$N \rightarrow N - \dot{f}N - f\dot{N} - \xi^i \partial_i N, \quad (15.71)$$

$$N_i \rightarrow N_i - \dot{f}N_i - f\dot{N}_i - \dot{\xi}^j q_{ij} - \nabla_i \xi^j N_j - \xi^j \nabla_j N_i, \quad (15.72)$$

$$q_{ij} \rightarrow q_{ij} - f\dot{q}_{ij} - q_{ik} \nabla_j \xi^k - q_{jk} \nabla_i \xi^k. \quad (15.73)$$

If N depends on t alone, the transformation (15.71) induces only the time-dependent change $-\partial_t(fN)$. Hence the condition $N = N(t)$, which is called the projectability condition, can be compatible with the foliation-preserving diffeomorphism. In this case, the acceleration vector $a_j = D_j \ln N$ vanishes.

The symmetry (15.70) does not force to restrict N to depend on the time t only, but we can also consider a non-projectable version in which the lapse depends on both t and x^i . In the original projectable Hořava–Lifshitz gravity there are pathologies associated with instabilities of perturbations [20, 21], but this problem can be circumvented in the non-projectable version due to the presence of non-vanishing acceleration vector [22, 25].

In GR, the Einstein–Hilbert action in the ADM language is given by Eq. (15.34). Only the combination $\mathcal{S} - K^2$ of kinetic terms is allowed due to the gauge symmetry of GR. In Hořava–Lifshitz gravity, both $\mathcal{S}$ and K^2 are invariant under the foliation-preserving diffeomorphism (15.70). Hence the kinetic action of this theory is given by

$$S_K = \frac{M_{\text{pl}}^2}{2} \int dt d^3x N \sqrt{q} (\mathcal{S} - \lambda K^2), \quad (15.74)$$

where λ is an arbitrary constant recovering the kinetic term of GR for $\lambda = 1$.

The potential term $\mathcal{R}$ in the Einstein–Hilbert action (15.34) contains second derivatives of q_{ij} with respect to the spatial coordinate x^i , whereas $\mathcal{S}$ and K^2 possess second time derivatives of q_{ij} . Under the $z = 1$ scaling ($t \rightarrow ct$ and $x^i \rightarrow cx^i$), the term $\mathcal{R}$ scales in the same way as $\mathcal{S}$ and K^2 . To realize the $z = 3$ scaling, we need to take into account terms containing six spatial derivatives like $\mathcal{Z}_1$ and $\mathcal{Z}_2$ in Eq. (15.36). In the non-projectable Hořava–Lifshitz gravity the acceleration $a_j = D_j \ln N$ does not vanish, so the terms like α_4 and α_5 in Eq. (15.37) exhibit

the $z = 3$ scaling as well. Hence the action of “potential” terms invariant under the $z = 3$ scaling is

$$S_{\mathcal{V}_3} = -\frac{1}{2M_{\text{pl}}^2} \int dt d^3x N \sqrt{q} (g_4 \mathcal{Z}_1 + g_5 \mathcal{Z}_2 + \eta_4 \alpha_4 + \eta_5 \alpha_5), \quad (15.75)$$

where g_4, g_5, η_4, η_5 are dimensionless constants. In the following, we do not take into account the terms irrelevant to the discussion of linear cosmological perturbations on the flat FLRW background (like $\mathcal{R}^3$).

The actions corresponding to the $z = 2$ and $z = 1$ scalings are given, respectively, by

$$S_{\mathcal{V}_2} = -\frac{1}{2} \int dt d^3x N \sqrt{q} (g_2 \mathcal{R}^2 + g_3 \mathcal{Z} + \eta_2 \alpha_2 + \eta_3 \alpha_3), \quad (15.76)$$

$$S_{\mathcal{V}_1} = \frac{M_{\text{pl}}^2}{2} \int dt d^3x N \sqrt{q} (\mathcal{R} + \eta_1 \alpha_1), \quad (15.77)$$

where $g_2, g_3, \eta_1, \eta_2, \eta_3$ are dimensionless constants. Taking the sum of Eqs. (15.74), (15.75), (15.76) and (15.77), the action of Hořava–Lifshitz gravity is given by $S = \int dt d^3x N \sqrt{q} \mathcal{L}$ with the Lagrangian density

$$\begin{aligned} \mathcal{L} = \frac{M_{\text{pl}}^2}{2} \left[S - \lambda K^2 + \mathcal{R} + \eta_1 \alpha_1 - M_{\text{pl}}^{-2} (g_2 \mathcal{R}^2 + g_3 \mathcal{Z} + \eta_2 \alpha_2 + \eta_3 \alpha_3) \right. \\ \left. - M_{\text{pl}}^{-4} (g_4 \mathcal{Z}_1 + g_5 \mathcal{Z}_2 + \eta_4 \alpha_4 + \eta_5 \alpha_5) \right], \end{aligned} \quad (15.78)$$

which depends on $K, S, \mathcal{R}, \mathcal{Z}, \mathcal{Z}_1, \mathcal{Z}_2, \alpha_i$ ($i = 1, 2, \dots, 5$). Hence Hořava–Lifshitz gravity can be encompassed in the EFT framework given by the action (15.38).

15.3. Cosmological perturbations

We expand the action (15.38) up to second order in scalar and tensor perturbations in the presence of a perfect fluid. For the perfect fluid we consider the k-essence Lagrangian $P(Y)$ that depends on the kinetic energy $Y = -g^{\mu\nu} \nabla_\mu \chi \nabla_\nu \chi / 2$ of a scalar field χ . The total action under consideration is given by

$$S = \int d^4x \sqrt{-g} [\mathcal{L}(N, K, S, \mathcal{R}, \mathcal{U}, \mathcal{Z}, \mathcal{Z}_1, \mathcal{Z}_2, \alpha_1, \dots, \alpha_5; t) + P(Y)]. \quad (15.79)$$

We consider the perturbed line element with four scalar metric perturbations δN , ψ , ζ , and E , as

$$ds^2 = -(1 + 2\delta N)dt^2 + 2\psi_{|i} dt dx^i + a^2(t) [(1 + 2\zeta)\delta_{ij} + 2E_{|ij}] dx^i dx^j. \quad (15.80)$$

As we discussed in Chap. 6, under the infinitesimal gauge transformation $t \rightarrow t + f(t, x^i)$ and $x^i \rightarrow x^i + \delta^{ij} \xi(t, x^i)_{|j}$, the perturbations δN and E transform as $\delta N \rightarrow$

$\delta N - \dot{f}$ and $E \rightarrow E - \xi$, respectively. By choosing the gauge

$$E = 0, \quad (15.81)$$

the spatial threading is fixed.

In Horndeski and GLPV theories, the temporal gauge-transformation vector is fixed by choosing the unitary gauge $\delta\phi = 0$, so we can employ the EFT approach based on the action (15.79) as if no scalar-field perturbations are present. For this gauge choice, the propagating scalar degree of freedom manifests itself through scalar metric perturbations.

In the projectable Hořava–Lifshitz gravity, the lapse N depends on t alone, so the perturbation δN vanishes. The fact that $\delta N = 0$ is consistent with the foliation-preserving transformation $t \rightarrow t + f(t)$. In the non-projectable Hořava–Lifshitz gravity, the lapse N depends on both x^i and t . If we choose the gauge $\delta N = 0$, this is inconsistent with the foliation-preserving transformation because the function f depends on x^i for this gauge choice. Without fixing the temporal gauge transformation, it is still possible to study the evolution of cosmological perturbations by appropriately constructing gauge-invariant variables.

We consider the flat FLRW background with the line element $ds^2 = -\bar{N}^2 dt^2 + a^2(t)\delta_{ij}dx^i dx^j$, where the background value of the lapse is $\bar{N} = 1$. From Eq. (15.16) the extrinsic curvature is given by $\bar{K}_{ij} = H\bar{q}_{ij}$, where $H = \dot{a}/a$ and a bar represents background values. The intrinsic curvature simply reduces to $\bar{\mathcal{R}}_{ij} = 0$. Then, the geometric scalar quantities yield

$$\begin{aligned} \bar{K} &= 3H, & \bar{\mathcal{S}} &= 3H^2, & \bar{\mathcal{R}} &= \bar{\mathcal{Z}} = \bar{\mathcal{U}} = 0, & \bar{\mathcal{Z}}_1 &= \bar{\mathcal{Z}}_2 = 0, \\ \bar{\alpha}_1 &= \bar{\alpha}_2 = \cdots = \bar{\alpha}_5 = 0. \end{aligned} \quad (15.82)$$

We define the perturbations of $K_{\mu\nu}$ and K as

$$\delta K_{\mu\nu} \equiv K_{\mu\nu} - Hq_{\mu\nu}, \quad (15.83)$$

$$\delta K \equiv K - 3H. \quad (15.84)$$

From the definition of $\mathcal{S}$ and Eq. (15.83), the perturbation $\delta\mathcal{S} \equiv \mathcal{S} - 3H^2$ can be written as

$$\delta\mathcal{S} = 2H\delta K + \delta K_\nu^\mu \delta K_\mu^\nu. \quad (15.85)$$

The quantities $\mathcal{R}$ and $\mathcal{Z}$ arise only as perturbations. Up to quadratic order, they can be expressed as

$$\delta\mathcal{R} = \delta_1\mathcal{R} + \delta_2\mathcal{R}, \quad \delta\mathcal{Z} = \delta\mathcal{R}_\nu^\mu \delta\mathcal{R}_\mu^\nu, \quad (15.86)$$

where $\delta_1\mathcal{R}$ and $\delta_2\mathcal{R}$ are first-order and second-order perturbations, respectively. The perturbation $\delta\mathcal{Z}$ is a second-order quantity. From Eq. (15.83), we find

$$\mathcal{U} = H\mathcal{R} + \mathcal{R}_\nu^\mu \delta K_\mu^\nu. \quad (15.87)$$

The first term on the right hand side of Eq. (15.87) contains the first-order contribution ($H\delta_1\mathcal{R}$) and the second-order contribution ($H\delta_2\mathcal{R}$), whereas the second term on the right hand side of Eq. (15.87) is a second-order quantity. From Eqs. (15.36) and (15.37), the quantities $\mathcal{Z}_1$, $\mathcal{Z}_2$, α_i ($i = 1, 2, \dots, 5$) are of second order in perturbations.

As for the matter sector, we decompose the field χ into the background and perturbed parts, as $\chi = \bar{\chi}(t) + \delta\chi(t, \mathbf{x})$. In the following, we omit the bar from the background value of χ . On using Eq. (15.6), we can expand the kinetic term $Y = -g^{\mu\nu}\nabla_\mu\chi\nabla_\nu\chi/2$, as

$$Y = \frac{1}{2}\dot{\chi}^2 + \delta_1 Y + \delta_2 Y, \quad (15.88)$$

where

$$\delta_1 Y = \dot{\chi}\delta\dot{\chi} - \dot{\chi}^2\delta N, \quad (15.89)$$

$$\delta_2 Y = \frac{1}{2}\delta\dot{\chi}^2 + \frac{3}{2}\dot{\chi}^2\delta N^2 - 2\dot{\chi}\delta\dot{\chi}\delta N - \frac{\dot{\chi}}{a^2}\partial_i\psi\partial_i\delta\chi - \frac{1}{2a^2}(\partial\delta\chi)^2, \quad (15.90)$$

where $(\partial\delta\chi)^2 \equiv \partial_i\delta\chi\partial_i\delta\chi$. Here, the quantities with same lower indices are summed over. Up to second order in perturbations, the Lagrangian density $P(Y)$ reads

$$P(Y) = \bar{P} + P_{,Y}(\delta_1 Y + \delta_2 Y) + \frac{P_{,YY}}{2}\delta_1 Y^2 + \mathcal{O}(3), \quad (15.91)$$

where a comma represents a partial derivative with respect to the corresponding subscript.

Expanding Eq. (15.79) up to second order in perturbations, the resulting action is given by $S = \int d^4x\sqrt{-g}\mathcal{L}_{\text{total}}$ with the Lagrangian density

$$\begin{aligned} \mathcal{L}_{\text{total}} = & \bar{\mathcal{L}} + \bar{P} + \mathcal{L}_{,N}\delta N + \mathcal{L}_{,K}\delta K + \mathcal{L}_{,S}\delta S + \mathcal{L}_{,\mathcal{R}}\delta\mathcal{R} + \mathcal{L}_{,\mathcal{Z}}\delta\mathcal{Z} + \mathcal{L}_{,\mathcal{U}}\delta\mathcal{U} + P_{,Y}\delta_1 Y \\ & + \frac{1}{2}\left(\delta N\frac{\partial}{\partial N} + \delta K\frac{\partial}{\partial K} + \delta S\frac{\partial}{\partial S} + \delta\mathcal{R}\frac{\partial}{\partial\mathcal{R}} + \delta\mathcal{U}\frac{\partial}{\partial\mathcal{U}}\right)^2 \mathcal{L} \\ & + P_{,Y}\delta_2 Y + \frac{P_{,YY}}{2}\delta_1 Y^2 + \sum_{i=1}^2 \mathcal{L}_{,\mathcal{Z}_i}\delta\mathcal{Z}_i + \sum_{i=1}^5 \mathcal{L}_{,\alpha_i}\delta\alpha_i + \mathcal{O}(3). \end{aligned} \quad (15.92)$$

There are also perturbations arising from the volume factor $\sqrt{-g} = N\sqrt{q}$.

15.3.1. Background equations of motion

We first compute the first-order contribution to Eq. (15.92) to derive the background equations of motion. On using Eqs. (15.84) and (15.85), it follows that

$$\mathcal{L}_{,K}\delta K + \mathcal{L}_{,S}\delta S = \mathcal{F}(K - 3H) + \mathcal{L}_{,S}\delta K^\mu_\nu\delta K^\nu_\mu, \quad (15.93)$$

where

$$\mathcal{F} \equiv \mathcal{L}_{,K} + 2H\mathcal{L}_{,S}. \quad (15.94)$$

From the definition (15.11) of the extrinsic curvature, it follows that $K = g^{\mu\nu} K_{\mu\nu} = q^{\mu\nu} \nabla_\mu n_\nu$. Substituting $q^{\mu\nu} = g^{\mu\nu} + n^\mu n^\nu$ and using $n^\mu n^\nu \nabla_\mu n_\nu = 0$, we have that $K = \nabla_\mu n^\mu$. Then, we can integrate the term $\mathcal{F}K$ in Eq. (15.93) by parts (up to a boundary term) as

$$\int d^4x \sqrt{-g} \mathcal{F}K = - \int d^4x \sqrt{-g} (\nabla_\mu \mathcal{F}) n^\mu = - \int d^4x \sqrt{-g} \frac{\dot{\mathcal{F}}}{N}, \quad (15.95)$$

which contains the lapse $N = 1 + \delta N$. Up to second order in perturbations, Eq. (15.93) reduces to

$$\mathcal{L}_{,K} \delta K + \mathcal{L}_{,S} \delta S = -\dot{\mathcal{F}} - 3H\mathcal{F} + \dot{\mathcal{F}} \delta N - \dot{\mathcal{F}} \delta N^2 + \mathcal{L}_{,S} \delta K_\nu^\mu \delta K_\mu^\nu + \mathcal{O}(3). \quad (15.96)$$

In Eq. (15.92), the first-order contribution to $\mathcal{L}_{,\mathcal{R}} \delta \mathcal{R}$ is given by $\mathcal{L}_{,\mathcal{R}} \delta_1 \mathcal{R}$, whereas $\mathcal{L}_{,\mathcal{Z}} \delta \mathcal{Z}$ is of second order. As for the term $\mathcal{L}_{,\mathcal{U}} \delta \mathcal{U}$, we employ the following relation [10]:

$$\int d^4x \sqrt{-g} \lambda(t) \mathcal{U} = \int d^4x \sqrt{-g} \left[\frac{\lambda(t)}{2} \mathcal{R}K + \frac{\dot{\lambda}(t)}{2N} \mathcal{R} \right], \quad (15.97)$$

which holds for a time-dependent function $\lambda(t)$ up to boundary terms. To prove this relation, we need to show that the integral

$$\mathcal{I} = \int d^4x \sqrt{-g} \left[\lambda(t) \mathcal{U} - \frac{\lambda(t)}{2} \mathcal{R}K - \frac{\dot{\lambda}(t)}{2N} \mathcal{R} \right], \quad (15.98)$$

reduces to boundary terms. On using the relations $K = \nabla_\mu n^\mu$, $n^\mu = -Ng^{0\mu}$, and Eq. (15.16), the integral (15.98) reduces to

$$\begin{aligned} \mathcal{I} &= \int d^4x \sqrt{-g} \lambda(t) \left(\mathcal{R}_{\mu\nu} K^{\mu\nu} + \frac{1}{2} n^\mu \nabla_\mu \mathcal{R} \right) \\ &= \int d^4x \sqrt{q} \lambda(t) \left[\frac{1}{2} \left(q^{ik} q^{jl} \dot{q}_{kl} \mathcal{R}_{ij} + \dot{\mathcal{R}} \right) - D^i N^j \mathcal{R}_{ij} - \frac{1}{2} N^i D_i \mathcal{R} \right] \\ &= \int d^4x \sqrt{q} \lambda(t) \left[\frac{1}{2} q^{ij} \dot{\mathcal{R}}_{ij} + N^j D^i {}^{(3)}G_{ij} \right], \end{aligned} \quad (15.99)$$

up to boundary terms. The three-dimensional Einstein tensor ${}^{(3)}G_{ij}$ obeys the Bianchi identity $D^i {}^{(3)}G_{ij} = 0$, so the second term on the right hand side of Eq. (15.99) vanishes. As we showed in Eq. (3.90), the term $q^{ij} \dot{\mathcal{R}}_{ij}$ in Eq. (15.99)

reduces to a boundary term of the form $D_i A^i$ in three dimensions. Hence we proved that the relation (15.97) holds up to boundary terms. Then, the term $\mathcal{L}_{,\mathcal{U}}\delta\mathcal{U}$ yields

$$\begin{aligned}\mathcal{L}_{,\mathcal{U}}\delta\mathcal{U} &= \frac{1}{2} \left(\dot{\mathcal{L}}_{,\mathcal{U}} + 3H\mathcal{L}_{,\mathcal{U}} \right) \delta_1\mathcal{R} + \frac{1}{2} \left(\dot{\mathcal{L}}_{,\mathcal{U}} + 3H\mathcal{L}_{,\mathcal{U}} \right) \delta_2\mathcal{R} \\ &+ \frac{1}{2} \left(\mathcal{L}_{,\mathcal{U}}\delta K - \dot{\mathcal{L}}_{,\mathcal{U}}\delta N \right) \delta_1\mathcal{R} + \mathcal{O}(3).\end{aligned}\quad (15.100)$$

Collecting zeroth and first-order contributions to Eq. (15.92), the action is given by $S = \int d^4x \sqrt{-g} \mathcal{L}_{\text{total}}$ with the Lagrangian density

$$\mathcal{L}_{\text{total}} = \bar{\mathcal{L}} + \bar{P} - \dot{\mathcal{F}} - 3H\mathcal{F} + (\dot{\mathcal{F}} + \mathcal{L}_{,N})\delta N + \mathcal{E}\delta_1\mathcal{R} + P_{,Y} \left(\dot{\chi}\delta\chi - \dot{\chi}^2\delta N \right) + \mathcal{O}(2), \quad (15.101)$$

where

$$\mathcal{E} \equiv \mathcal{L}_{,\mathcal{R}} + \frac{1}{2}\dot{\mathcal{L}}_{,\mathcal{U}} + \frac{3}{2}H\mathcal{L}_{,\mathcal{U}}. \quad (15.102)$$

Defining $L \equiv \sqrt{-g}\mathcal{L}_{\text{total}} = N\sqrt{q}\mathcal{L}_{\text{total}}$, the zeroth-order and first-order Lagrangian contributions to L are given, respectively, by

$$L_0 = a^3(\bar{\mathcal{L}} - \dot{\mathcal{F}} - 3H\mathcal{F} + \bar{P}), \quad (15.103)$$

$$\begin{aligned}L_1 &= a^3 \left(\bar{\mathcal{L}} + \mathcal{L}_{,N} - 3H\mathcal{F} + \bar{P} - P_{,Y}\dot{\chi}^2 \right) \delta N + \left(\bar{\mathcal{L}} - \dot{\mathcal{F}} - 3H\mathcal{F} + \bar{P} \right) \delta\sqrt{q} \\ &+ a^3 P_{,Y}\dot{\chi}\delta\chi + a^3 \mathcal{E}\delta_1\mathcal{R}.\end{aligned}\quad (15.104)$$

The last term on the right hand side of Eq. (15.104) is a total derivative, so it does not contribute to the background equations of motion. Varying the first-order Lagrangian (15.104) with respect to δN , $\delta\sqrt{q}$, and $\delta\chi$, respectively, we obtain

$$\bar{\mathcal{L}} + \mathcal{L}_{,N} - 3H\mathcal{F} = \rho, \quad (15.105)$$

$$\bar{\mathcal{L}} - \dot{\mathcal{F}} - 3H\mathcal{F} = -P, \quad (15.106)$$

$$\frac{d}{dt} (a^3 P_{,Y}\dot{\chi}) = 0, \quad (15.107)$$

where we omitted the bar from the pressure P , and the matter density is given by $\rho = P_{,Y}\dot{\chi}^2 - P$. From Eq. (15.106), the zeroth order Lagrangian (15.103) vanishes identically. Combining Eq. (15.105) with Eq. (15.106), it follows that

$$\mathcal{L}_{,N} + \dot{\mathcal{F}} = \rho + P. \quad (15.108)$$

As we showed in Eq. (15.34), the Lagrangian density of GR is given by $\mathcal{L} = (M_{\text{pl}}^2/2)(\mathcal{R} - K^2 + \mathcal{S})$. Since in this case $\bar{\mathcal{L}} = -3M_{\text{pl}}^2 H^2$, $\mathcal{L}_{,N} = 0$, and $\mathcal{F} = -2M_{\text{pl}}^2 H$, Eqs. (15.105) and (15.108) reduce, respectively, to $3M_{\text{pl}}^2 H^2 = \rho$ and $-2M_{\text{pl}}^2 \dot{H} = \rho + P$. We need to caution that, for the theories in which the lapse N depends on t alone (i.e., $\delta N = 0$), it is not allowed to take a variation with respect to δN . This happens for the projectable version of Hořava Lifshitz gravity, so we will discuss such cases separately in Sec. 15.5.

15.3.2. Linear perturbation equations of motion

We expand the action (15.79) up to second order in perturbations to derive linear linear perturbation equations of motion. Using Eqs. (15.91), (15.96) and (15.100), the total action is given by $S = \int d^4x \sqrt{-g} \mathcal{L}_{\text{total}}$ with the Lagrangian density

$$\begin{aligned} \mathcal{L}_{\text{total}} = & \bar{\mathcal{L}} + \bar{P} - \dot{\mathcal{F}} - 3H\mathcal{F} + (\dot{\mathcal{F}} + \mathcal{L}_{,N})\delta N + \mathcal{E}\delta_1\mathcal{R} + P_{,Y}\delta_1Y \\ & + \left(\frac{\mathcal{L}_{,NN}}{2} - \dot{\mathcal{F}} \right) \delta N^2 + \frac{1}{2}\mathcal{A}\delta K^2 + \mathcal{B}\delta K\delta N + \mathcal{C}\delta K\delta_1\mathcal{R} + \mathcal{D}\delta N\delta_1\mathcal{R} + \mathcal{E}\delta_2\mathcal{R} \\ & + \frac{1}{2}\mathcal{G}\delta_1\mathcal{R}^2 + \mathcal{L}_{,S}\delta K_\nu^\mu\delta K_\mu^\nu + \mathcal{L}_{,\mathcal{Z}}\delta\mathcal{R}_\nu^\mu\delta\mathcal{R}_\mu^\nu + \sum_{i=1}^2 \mathcal{L}_{,\mathcal{Z}_i}\delta\mathcal{Z}_i + \sum_{i=1}^5 \mathcal{L}_{,\alpha_i}\delta\alpha_i \\ & + P_{,Y}\delta_2Y + \frac{P_{,YY}}{2}\delta_1Y^2 + \mathcal{O}(3), \end{aligned} \quad (15.109)$$

where

$$\mathcal{A} = \mathcal{L}_{,KK} + 4H\mathcal{L}_{,SK} + 4H^2\mathcal{L}_{,SS}, \quad (15.110)$$

$$\mathcal{B} = \mathcal{L}_{,KN} + 2H\mathcal{L}_{,SN}, \quad (15.111)$$

$$\mathcal{C} = \mathcal{L}_{,K\mathcal{R}} + 2H\mathcal{L}_{,S\mathcal{R}} + \frac{1}{2}\mathcal{L}_{,\mathcal{U}} + H\mathcal{L}_{,K\mathcal{U}} + 2H^2\mathcal{L}_{,S\mathcal{U}}, \quad (15.112)$$

$$\mathcal{D} = \mathcal{L}_{,N\mathcal{R}} - \frac{1}{2}\dot{\mathcal{L}}_{,\mathcal{U}} + H\mathcal{L}_{,N\mathcal{U}}, \quad (15.113)$$

$$\mathcal{G} = \mathcal{L}_{,\mathcal{R}\mathcal{R}} + 2H\mathcal{L}_{,\mathcal{R}\mathcal{U}} + H^2\mathcal{L}_{,\mathcal{U}\mathcal{U}}. \quad (15.114)$$

Writing first-order and second-order Lagrangians of Eq. (15.109) as $\mathcal{L}_1$ and $\mathcal{L}_2$, respectively, the second-order action is given by $S_2 = \int d^4x L_2$, with $L_2 = a^3\delta N\mathcal{L}_1 + \delta\sqrt{q}\mathcal{L}_1 + a^3\mathcal{L}_2$. Note that the second-order contribution arising from the expansion of $\sqrt{-g}$ is multiplied by the zeroth-order Lagrangian (15.103), so it vanishes identically from Eq. (15.106). Then, it follows that

$$\begin{aligned} L_2 = & \delta\sqrt{q} \left[(\dot{\mathcal{F}} + \mathcal{L}_{,N})\delta N + \mathcal{E}\delta_1\mathcal{R} + P_{,Y}\delta_1Y \right] \\ & + a^3 \left[\left(\mathcal{L}_{,N} + \frac{\mathcal{L}_{,NN}}{2} \right) \delta N^2 + \mathcal{E}\delta_2\mathcal{R} + \frac{1}{2}\mathcal{A}\delta K^2 + \mathcal{B}\delta K\delta N + \mathcal{C}\delta K\delta_1\mathcal{R} \right. \\ & + (\mathcal{D} + \mathcal{E})\delta N\delta_1\mathcal{R} + \frac{1}{2}\mathcal{G}\delta_1\mathcal{R}^2 + \mathcal{L}_{,S}\delta K_\nu^\mu\delta K_\mu^\nu + \mathcal{L}_{,\mathcal{Z}}\delta\mathcal{R}_\nu^\mu\delta\mathcal{R}_\mu^\nu + \sum_{i=1}^2 \mathcal{L}_{,\mathcal{Z}_i}\delta\mathcal{Z}_i \\ & \left. + \sum_{i=1}^5 \mathcal{L}_{,\alpha_i}\delta\alpha_i + P_{,Y}(\delta N\delta_1Y + \delta_2Y) + \frac{P_{,YY}}{2}\delta_1Y^2 \right]. \end{aligned} \quad (15.115)$$

The perturbations of extrinsic and intrinsic curvatures can be expressed in terms of metric perturbations δN , ψ , and ζ . Since $q_{ij} = a^2(t)(1 + 2\zeta)\delta_{ij}$ for the gauge

choice (15.81), the perturbation $\delta\sqrt{q}$ in Eq. (15.115) is equivalent to $3a^3\zeta$. At first order, the extrinsic curvature (15.16) is

$$\delta K_j^i = (\dot{\zeta} - H\delta N)\delta_j^i - \frac{1}{2a^2}\delta^{ik}(\partial_k N_j + \partial_j N_k). \quad (15.116)$$

Since the Christoffel symbols Γ_{ij}^k are first-order in perturbations, the three-dimensional derivatives like $\nabla_i N_j$ were replaced with partial derivatives like $\partial_i N_j$ in Eq. (15.116). Taking the trace of Eq. (15.116) and using $N_i = \partial_i \psi$, we obtain

$$\delta K = 3(\dot{\zeta} - H\delta N) - \Delta\psi, \quad (15.117)$$

where the operator Δ is given by

$$\Delta = \nabla_i \nabla^i = a^{-2}(t)\delta^{ij}\partial_i \partial_j \equiv a^{-2}(t)\partial^2. \quad (15.118)$$

The perturbations associated with the intrinsic curvature are given by

$$\delta\mathcal{R}_{ij} = -(\delta_{ij}\partial^2\zeta + \partial_i\partial_j\zeta), \quad (15.119)$$

$$\delta_1\mathcal{R} = -4a^{-2}\partial^2\zeta, \quad (15.120)$$

$$\delta_2\mathcal{R} = -2a^{-2}[(\partial\zeta)^2 - 4\zeta\partial^2\zeta], \quad (15.121)$$

where $(\partial\zeta)^2 \equiv \delta^{ij}(\partial_i\zeta)(\partial_j\zeta)$. The terms $\mathcal{L}_{,\mathcal{Z}_1}\delta\mathcal{Z}_1$ and $\mathcal{L}_{,\mathcal{Z}_2}\delta\mathcal{Z}_2$ are computed as

$$\begin{aligned} \mathcal{L}_{,\mathcal{Z}_1}\delta\mathcal{Z}_1 &= \mathcal{L}_{,\mathcal{Z}_1}(\nabla^i\delta_1\mathcal{R})(\nabla_i\delta_1\mathcal{R}) = 16\mathcal{L}_{,\mathcal{Z}_1}(\nabla^i\Delta\zeta)(\nabla_i\Delta\zeta) = 16\mathcal{L}_{,\mathcal{Z}_1}(\Delta\partial^i\zeta)(\Delta\partial_i\zeta), \\ \mathcal{L}_{,\mathcal{Z}_2}\delta\mathcal{Z}_2 &= \mathcal{L}_{,\mathcal{Z}_2}(h_{jk}\Delta\partial_i\zeta + \partial_i\partial_j\partial_k\zeta)(h^{jk}\Delta\partial^i\zeta + \partial^i\partial^j\partial^k\zeta) = 6\mathcal{L}_{,\mathcal{Z}_2}(\Delta\partial^i\zeta)(\Delta\partial_i\zeta), \end{aligned} \quad (15.122)$$

which are valid up to second order in perturbations and up to boundary terms. The perturbed quantities related to the acceleration vector yield

$$\begin{aligned} \mathcal{L}_{,\alpha_1}\delta\alpha_1 &= \mathcal{L}_{,\alpha_1}(\partial_i\delta N)(\partial^i\delta N), \\ \mathcal{L}_{,\alpha_2}\delta\alpha_2 &= \mathcal{L}_{,\alpha_2}(\partial_i\delta N)\Delta(\partial^i\delta N), \\ \mathcal{L}_{,\alpha_3}\delta\alpha_3 &= 4\mathcal{L}_{,\alpha_3}(\partial_i\delta N)\Delta(\partial^i\zeta), \\ \mathcal{L}_{,\alpha_4}\delta\alpha_4 &= \mathcal{L}_{,\alpha_4}\Delta(\partial_i\delta N)\Delta(\partial^i\delta N), \\ \mathcal{L}_{,\alpha_5}\delta\alpha_5 &= 4\mathcal{L}_{,\alpha_5}\Delta(\partial_i\delta N)\Delta(\partial^i\zeta). \end{aligned} \quad (15.123)$$

Substituting Eqs. (15.116), (15.117), (15.121)–(15.123) into Eq. (15.115) and using the background equation (15.108), it follows that

$$\begin{aligned} L_2 &= a^3 \left\{ \frac{1}{2} [2\mathcal{L}_{,N} + \mathcal{L}_{,NN} - 6H\mathcal{W} - 3H^2(3\mathcal{A} + 2\mathcal{L}_{,S})] \delta N^2 + [\mathcal{W}(3\dot{\zeta} - \Delta\psi) \right. \\ &\quad \left. + 4(3HC - \mathcal{D} - \mathcal{E})\Delta\zeta]\delta N - (3\mathcal{A} + 2\mathcal{L}_{,S})\dot{\zeta}\Delta\psi - 12\mathcal{C}\dot{\zeta}\Delta\zeta + \left(\frac{9}{2}\mathcal{A} + 3\mathcal{L}_{,S}\right)\dot{\zeta}^2 \right. \end{aligned}$$

$$\begin{aligned}
& + 2\mathcal{E}\frac{(\partial\zeta)^2}{a^2} + \frac{1}{2}(\mathcal{A} + 2\mathcal{L}_{,S})(\Delta\psi)^2 + 4\mathcal{C}(\Delta\psi)(\Delta\zeta) + 2(4\mathcal{G} + 3\mathcal{L}_{,Z})(\Delta\zeta)^2 \\
& + 2(8\mathcal{L}_{,Z_1} + 3\mathcal{L}_{,Z_2})(\Delta\partial^i\zeta)(\Delta\partial_i\zeta) + \mathcal{L}_{,\alpha_1}(\partial_i\delta N)(\partial^i\delta N) + \mathcal{L}_{,\alpha_2}(\partial_i\delta N)\Delta(\partial^i\delta N) \\
& + 4\mathcal{L}_{,\alpha_3}(\partial_i\delta N)\Delta(\partial^i\zeta) + \mathcal{L}_{,\alpha_4}\Delta(\partial_i\delta N)\Delta(\partial^i\delta N) + 4\mathcal{L}_{,\alpha_5}\Delta(\partial_i\delta N)\Delta(\partial^i\zeta) \Big\} \\
& + L_m,
\end{aligned} \tag{15.124}$$

where

$$\mathcal{W} \equiv \mathcal{B} - 3AH - 2\mathcal{L}_{,S}H, \tag{15.125}$$

and L_m is the matter Lagrangian given by

$$\begin{aligned}
L_m = a^3 \Big[\frac{1}{2} (P_{,Y} + \dot{\chi}^2 P_{,YY}) \left(\dot{\chi}^2 \delta N^2 - 2\dot{\chi} \delta\dot{\chi} \delta N + \delta\dot{\chi}^2 \right) + 3\dot{\chi} P_{,Y} \zeta \dot{\chi} \\
+ \dot{\chi} P_{,Y} \delta\chi \Delta\psi - \frac{P_{,Y}}{2} \frac{(\partial\delta\chi)^2}{a^2} \Big].
\end{aligned} \tag{15.126}$$

The Lagrangian (15.124) contains spatial derivatives higher than second order, so the variation with respect to δN leads to

$$\frac{\partial L_2}{\partial(\delta N)} - \partial_i \left(\frac{\partial L_2}{\partial(\partial_i \delta N)} \right) + \partial_i \partial_j \left(\frac{\partial L_2}{\partial(\partial_i \partial_j \delta N)} \right) - \partial_i \partial_j \partial_k \left(\frac{\partial L_2}{\partial(\partial_i \partial_j \partial_k \delta N)} \right) + \dots = 0. \tag{15.127}$$

For example, the term $a^3 \mathcal{L}_{,\alpha_2}(\partial_i \delta N) \Delta(\partial^i \delta N)$ equals to $-a^3 \mathcal{L}_{,\alpha_2}(\partial_i \partial_j \delta N)^2 / a^4$ up to a boundary term, so the third term on the left hand side of (15.127) gives $-2a^3 \mathcal{L}_{,\alpha_2} \Delta^2 \delta N$.

Varying the Lagrangian (15.124) with respect to δN and ψ , respectively, we obtain the Hamiltonian and momentum constraints, as

$$\begin{aligned}
& [2\mathcal{L}_{,N} + \mathcal{L}_{,NN} - 6H\mathcal{W} - 3H^2(3\mathcal{A} + 2\mathcal{L}_{,S})] \delta N + \mathcal{W}(3\dot{\zeta} - \Delta\psi) \\
& + 4(3H\mathcal{C} - \mathcal{D} - \mathcal{E})\Delta\zeta - 2\mathcal{L}_{,\alpha_1}\Delta\delta N - 2\mathcal{L}_{,\alpha_2}\Delta^2\delta N - 4\mathcal{L}_{,\alpha_3}\Delta^2\zeta \\
& - 2\mathcal{L}_{,\alpha_4}\Delta^3\delta N - 4\mathcal{L}_{,\alpha_5}\Delta^3\zeta \\
& = \delta\rho,
\end{aligned} \tag{15.128}$$

$$\mathcal{W}\delta N + (3\mathcal{A} + 2\mathcal{L}_{,S})\dot{\zeta} - 4\mathcal{C}\Delta\zeta - (\mathcal{A} + 2\mathcal{L}_{,S})\Delta\psi = -\delta q, \tag{15.129}$$

where $\delta\rho$ and δq are density and momentum perturbations of matter given by

$$\delta\rho \equiv (P_{,Y} + \dot{\chi}^2 P_{,YY}) \left(\dot{\chi} \delta\dot{\chi} - \dot{\chi}^2 \delta N \right), \tag{15.130}$$

$$\delta q \equiv -P_{,Y} \dot{\chi} \delta\chi. \tag{15.131}$$

Variation of (15.124) with respect to ζ leads to

$$\begin{aligned} \dot{\mathcal{Y}} + 3H\mathcal{Y} - 4(3HC - \mathcal{D} - \mathcal{E})\Delta\delta N + 4\mathcal{E}\Delta\zeta + 12\mathcal{C}\Delta\dot{\zeta} - 4\mathcal{C}\Delta^2\psi \\ - 4(4\mathcal{G} + 3\mathcal{L}_{,\mathcal{Z}})\Delta^2\zeta + 4(8\mathcal{L}_{,\mathcal{Z}_1} + 3\mathcal{L}_{,\mathcal{Z}_2})\Delta^3\zeta + 4\mathcal{L}_{,\alpha_3}\Delta^2\delta N \\ + 4\mathcal{L}_{,\alpha_5}\Delta^3\delta N \\ = 3\delta P + 3(\rho + P)\delta N, \end{aligned} \quad (15.132)$$

where we used $\dot{\chi}^2 P_{,\mathcal{Y}} = \rho + P$, and

$$\delta P \equiv P_{,\mathcal{Y}}\dot{\chi}\delta\chi - (\rho + P)\delta N, \quad (15.133)$$

$$\mathcal{Y} = 3 \left[\mathcal{W}\delta N + (3\mathcal{A} + 2\mathcal{L}_{,\mathcal{S}})\dot{\zeta} - 4\mathcal{C}\Delta\zeta \right] - (3\mathcal{A} + 2\mathcal{L}_{,\mathcal{S}})\Delta\psi. \quad (15.134)$$

From Eq. (15.129), the quantity (15.134) reduces to

$$\mathcal{Y} = 4\mathcal{L}_{,\mathcal{S}}\Delta\psi - 3\delta q = 4\mathcal{L}_{,\mathcal{S}}\frac{\partial^2\psi}{a^2} - 3\delta q, \quad (15.135)$$

so that $\dot{\mathcal{Y}} + 3H\mathcal{Y} = -3(\dot{\delta q} + 3H\delta q) + \Delta[4(\mathcal{L}_{,\mathcal{S}}\dot{\psi} + \dot{\mathcal{L}}_{,\mathcal{S}}\psi + H\mathcal{L}_{,\mathcal{S}}\psi)]$. On using the background equation (15.107), the momentum perturbation $\delta q = -P_{,\mathcal{Y}}\dot{\chi}\delta\chi$ obeys

$$\dot{\delta q} + 3H\delta q + \delta P + (\rho + P)\delta N = 0. \quad (15.136)$$

Then, we can write Eq. (15.132) in the following form

$$\begin{aligned} \Delta[\mathcal{L}_{,\mathcal{S}}\dot{\psi} + \dot{\mathcal{L}}_{,\mathcal{S}}\psi + H\mathcal{L}_{,\mathcal{S}}\psi + \mathcal{E}\zeta + 3\mathcal{C}\dot{\zeta} - (3HC - \mathcal{D} - \mathcal{E})\delta N - \mathcal{C}\Delta\psi \\ - (4\mathcal{G} + 3\mathcal{L}_{,\mathcal{Z}})\Delta\zeta + (8\mathcal{L}_{,\mathcal{Z}_1} + 3\mathcal{L}_{,\mathcal{Z}_2})\Delta^2\zeta + \mathcal{L}_{,\alpha_3}\Delta\delta N + \mathcal{L}_{,\alpha_5}\Delta^2\delta N] = 0. \end{aligned} \quad (15.137)$$

Varying the Lagrangian (15.124) with respect to ζ and using the definitions of $\delta\rho, \delta P, \delta q$, it follows that

$$\dot{\delta\rho} + 3H(\delta\rho + \delta P) + (\rho + P)(3\dot{\zeta} - \Delta\psi) + \Delta\delta q = 0. \quad (15.138)$$

The dynamics of scalar perturbations $\delta N, \psi, \zeta, \delta\chi$ is known by solving Eqs. (15.128), (15.129), (15.137) and (15.138) together with the background equations of motion (15.105)–(15.107).

15.4. Application to GLPV theories

In this section, we consider theories in which the equations of motion for linear cosmological perturbations on the flat FLRW background are of second order. As we will see below, this includes not only Horndeski theories but also GLPV theories.

In Eq. (15.132), higher-order spatial derivative terms are absent under the conditions $\mathcal{C} = 0$, $4\mathcal{G} + 3\mathcal{L}_{,\mathcal{Z}} = 0$, $8\mathcal{L}_{,\mathcal{Z}_1} + 3\mathcal{L}_{,\mathcal{Z}_2} = 0$, $\mathcal{L}_{,\alpha_3} = 0$, and $\mathcal{L}_{,\alpha_5} = 0$. Moreover, absence of higher-order derivatives in Eq. (15.128) requires that $\mathcal{L}_{,\alpha_2} = 0$

and $\mathcal{L}_{,\alpha_4} = 0$. From Eq. (15.129), the perturbation δN is related to the term $(\mathcal{A} + 2\mathcal{L}_{,\mathcal{S}})\Delta\psi$ for $\mathcal{W} \neq 0$. Then, the third term on the left hand side of Eq. (15.132) gives rise to the fourth-order spatial derivative $\Delta^2\psi$, so absence of this term requires that $\mathcal{A} + 2\mathcal{L}_{,\mathcal{S}} = 0$.

From Eq. (15.129), δN also depends on the term $(3\mathcal{A} + 2\mathcal{L}_{,\mathcal{S}})\dot{\zeta}$ for $\mathcal{W} \neq 0$. The third term on the left hand side of Eq. (15.132) gives rise to the combination of time and spatial derivatives $\Delta\dot{\zeta}$ higher than two, but as we will see below, this exactly cancels another term. On the other hand, unless $\mathcal{L}_{,\alpha_1} = 0$, the term $-2\mathcal{L}_{,\alpha_1}\Delta\delta N$ in Eq. (15.128) leads to the derivative higher than second order.

The above discussion shows that the equations of motion of linear cosmological perturbations are remain of second order under the conditions

$$\begin{aligned} \mathcal{C} = 0, \quad 4\mathcal{G} + 3\mathcal{L}_{,\mathcal{Z}} = 0, \quad \mathcal{A} + 2\mathcal{L}_{,\mathcal{S}} = 0, \quad 8\mathcal{L}_{,\mathcal{Z}_1} + 3\mathcal{L}_{,\mathcal{Z}_2} = 0, \\ \mathcal{L}_{,\alpha_1} = \mathcal{L}_{,\alpha_2} = \dots = \mathcal{L}_{,\alpha_5} = 0. \end{aligned} \quad (15.139)$$

Since the Lagrangian density (15.59) of GLPV theories satisfies the condition (15.139), the linear perturbation equations in GLPV theories are of second order. In this section, we consider theories satisfying the conditions (15.139).

In GLPV theories we have $\bar{K} = 3H$, $\bar{\mathcal{S}} = 3H^2$, $\bar{K}_3 = 6H^3$ and $\bar{\mathcal{R}} = \bar{\mathcal{U}} = 0$, so the background equations (15.105) and (15.106) reduce, respectively, to [26]

$$A_2 - 6H^2 A_4 - 12H^3 A_5 - \dot{\phi}^2 (A_{2,X} + 3H A_{3,X} + 6H^2 A_{4,X} + 6H^3 A_{5,X}) = \rho, \quad (15.140)$$

$$A_2 - 6H^2 A_4 - 12H^3 A_5 - \dot{A}_3 - 4\dot{H} A_4 - 4H \dot{A}_4 - 12H \dot{H} A_5 - 6H^2 \dot{A}_5 = -P, \quad (15.141)$$

which do not contain the functions B_4 and B_5 . This means that, at the background level, GLPV theories cannot be distinguished from Horndeski theories.

15.4.1. *Second-order action of scalar perturbations without matter*

First, we study the case in which the matter perfect fluid is absent ($\chi = 0$). Then, Eqs. (15.128), (15.129) and (15.137) reduce, respectively, to

$$(2\mathcal{L}_{,\mathcal{N}} + \mathcal{L}_{,\mathcal{N}\mathcal{N}} - 6H\mathcal{W} + 12H^2\mathcal{L}_{,\mathcal{S}})\delta N + \mathcal{W}(3\dot{\zeta} - \Delta\psi) - 4(\mathcal{D} + \mathcal{E})\Delta\zeta = 0, \quad (15.142)$$

$$\mathcal{W}\delta N - 4\mathcal{L}_{,\mathcal{S}}\dot{\zeta} = 0, \quad (15.143)$$

$$\frac{1}{a^3} \frac{d}{dt} (a^3 \mathcal{L}_{,\mathcal{S}} \Delta\psi) + \mathcal{E} \Delta\zeta + (\mathcal{D} + \mathcal{E}) \Delta\delta N = 0. \quad (15.144)$$

As long as $\mathcal{W} = \mathcal{L}_{,KN} + 2H\mathcal{L}_{,SN} + 4H\mathcal{L}_{,S} \neq 0$, it follows that $\delta N = 4\mathcal{L}_{,S}\dot{\zeta}/\mathcal{W}$ from Eq. (15.143). Substituting this relation into Eq. (15.142), we obtain

$$\Delta\psi = \frac{Q_s}{2\mathcal{L}_{,S}}\dot{\zeta} - \frac{4(\mathcal{D} + \mathcal{E})}{\mathcal{W}}\Delta\zeta, \quad (15.145)$$

where

$$Q_s \equiv \frac{2\mathcal{L}_{,S}}{3\mathcal{W}^2}(9\mathcal{W}^2 + 8\mathcal{L}_{,S}\xi), \quad (15.146)$$

with

$$\xi \equiv 3\mathcal{L}_{,N} + \frac{3}{2}\mathcal{L}_{,NN} - 9H\mathcal{W} + 18H^2\mathcal{L}_{,S}. \quad (15.147)$$

We express the terms $\Delta\delta N$ and $\Delta\psi$ in Eq. (15.144) with respect to ζ and its derivatives. Since the two terms $\Delta\dot{\zeta}$ cancel out, we obtain the equation of motion of ζ as

$$\frac{d}{dt}\left(a^3Q_s\dot{\zeta}\right) - aQ_sc_s^2\partial^2\zeta = 0, \quad (15.148)$$

where

$$c_s^2 \equiv \frac{2}{Q_s}(\dot{\mathcal{M}} + H\mathcal{M} - \mathcal{E}), \quad (15.149)$$

with

$$\mathcal{M} \equiv \frac{4\mathcal{L}_{,S}(\mathcal{D} + \mathcal{E})}{\mathcal{W}} = \frac{4\mathcal{L}_{,S}}{\mathcal{W}}\left(\mathcal{L}_{,\mathcal{R}} + \mathcal{L}_{,NR} + H\mathcal{L}_{,NU} + \frac{3}{2}H\mathcal{L}_{,U}\right). \quad (15.150)$$

Substituting the relations (15.143) and (15.145) into Eq. (15.124) for $\mathcal{W} \neq 0$, we obtain the second-order Lagrangian [10]

$$L_2 = a^3Q_s\left[\dot{\zeta}^2 - \frac{c_s^2}{a^2}(\partial\zeta)^2\right]. \quad (15.151)$$

Variation of the Lagrangian (15.151) with respect to ζ gives rise to Eq. (15.148). Hence there is one scalar propagating degree of freedom with second-order linear perturbation equations of motion. The conditions for the absence of ghosts and Laplacian instabilities correspond to $Q_s > 0$ and $c_s^2 > 0$, respectively. As we carried out in Sec. 6.8, the Lagrangian (15.151) can be applied to the computation of the primordial power spectrum of scalar perturbations for the single-field inflationary scenario in the framework of GLPV theories [27, 28].

15.4.2. Second-order action of tensor perturbations

In addition to the conditions $Q_s > 0$ and $c_s^2 > 0$, there are also theoretically consistent conditions associated with the stability of tensor perturbations for the theories satisfying Eq. (15.139). The three-dimensional metric q_{ij} containing divergence-free and traceless tensor perturbations h_{ij} (satisfying $h_{ij}{}^{[j} = 0$ and $h_i{}^i = 0$) can be written as

$$q_{ij} = a^2(t)(1 + 2\zeta)\hat{q}_{ij}, \quad \hat{q}_{ij} = \delta_{ij} + h_{ij} + \frac{1}{2}h_{ik}h_{kj}, \quad \det \hat{q} = 1, \quad (15.152)$$

where the term $h_{ik}h_{kj}/2$ was introduced for the simplification of calculations [29]. Tensor modes are decoupled from scalar modes at linear order in perturbations. The contribution arising from the tensor sector to perturbations of extrinsic and intrinsic curvatures are given by $\delta K = 0$, $\delta K_j^i = \delta^{ik}\dot{h}_{kj}/2$, $\delta_1\mathcal{R} = 0$, and $\delta_2\mathcal{R} = -(\partial h_{ij})^2/(4a^2)$. Hence the second-order action of tensor perturbations yields [10]

$$\begin{aligned} S_t^{(2)} &= \int d^4x a^3 \left[\mathcal{L}_{,S} \left(\delta K_i^j \delta K_j^i - \delta K^2 \right) + \mathcal{E} \delta_2 \mathcal{R} \right] \\ &= \int d^4x \frac{a^3}{4} \left[\mathcal{L}_{,S} \dot{h}_{ij}^2 - \frac{\mathcal{E}}{a^2} (\partial h_{ij})^2 \right]. \end{aligned} \quad (15.153)$$

Expressing h_{ij} as Eq. (6.153) with the two polarization tensors e_{ij}^+ and $e_{ij}^\times$, the action (15.153) reduces to

$$S_t^{(2)} = \sum_{\lambda=+,\times} \int dt d^3x a^3 Q_t \left[\dot{h}_\lambda^2 - \frac{c_t^2}{a^2} (\partial h_\lambda)^2 \right], \quad (15.154)$$

where

$$Q_t \equiv \frac{\mathcal{L}_{,S}}{2}, \quad c_t^2 \equiv \frac{\mathcal{E}}{\mathcal{L}_{,S}}. \quad (15.155)$$

The conditions for the absence of tensor ghosts and Laplacian instabilities correspond to $Q_t > 0$ and $c_t^2 > 0$, respectively. In GLPV theories, these conditions translate to

$$\mathcal{L}_{,S} = -A_4 - 3HA_5 > 0, \quad (15.156)$$

$$\mathcal{E} = B_4 + \frac{1}{2}\dot{B}_5 > 0. \quad (15.157)$$

The quantity $\mathcal{E}$ in the numerator of c_t^2 contains B_4 and B_5 , so it is possible to distinguish between GLPV and Horndeski theories, from the tensor propagation speed.

15.4.3. GLPV theories in the presence of matter

Now, we consider the case in which a single perfect fluid is present for theories satisfying the conditions (15.139). In this case, Eqs. (15.128) and (15.129) reduce, respectively, to

$$\begin{aligned} (2\mathcal{L}_{,N} + \mathcal{L}_{,NN} - 6H\mathcal{W} + 12H^2\mathcal{L}_{,S})\delta N + \mathcal{W}(3\dot{\zeta} - \Delta\psi) - 4(\mathcal{D} + \mathcal{E})\Delta\zeta \\ = (P_{,Y} + \dot{\chi}^2 P_{,YY})(\dot{\chi}\delta\dot{\chi} - \dot{\chi}^2\delta N), \end{aligned} \quad (15.158)$$

$$\mathcal{W}\delta N - 4\mathcal{L}_{,S}\dot{\zeta} = P_{,Y}\dot{\chi}\delta\chi. \quad (15.159)$$

We solve Eqs. (15.158) and (15.159) for δN and $\Delta\psi$ and substitute them into the Lagrangian (15.124). Then, the second-order action $S_2 = \int d^4x L_2$ reduces to the form (12.66) with the 2×2 matrices $\mathbf{K}$, $\mathbf{G}$, $\mathbf{B}$, $\mathbf{M}$ and the dimensionless vector field

$$\vec{\mathcal{A}}^t = (\zeta, \delta\chi/M_{\text{pl}}). \quad (15.160)$$

The components of $\mathbf{K}$ and $\mathbf{G}$, which are associated with no-ghost and stability conditions of scalar perturbations, read

$$\begin{aligned} K_{11} &= Q_s + \frac{16\mathcal{L}_{,S}^2}{M_{\text{pl}}^2\mathcal{W}^2}\dot{\chi}^2 K_{22}, & K_{22} &= \frac{1}{2}(P_{,Y} + \dot{\chi}^2 P_{,YY})M_{\text{pl}}^2, \\ K_{12} &= K_{21} = -\frac{4\mathcal{L}_{,S}\dot{\chi}}{M_{\text{pl}}\mathcal{W}}K_{22}, & G_{11} &= 2(\dot{\mathcal{M}} + H\mathcal{M} - \mathcal{E}), \\ G_{22} &= \frac{1}{2}P_{,Y}M_{\text{pl}}^2, & G_{12} &= G_{21} = -\frac{\mathcal{M}\dot{\chi}}{\mathcal{L}_{,S}M_{\text{pl}}}G_{22}, \end{aligned} \quad (15.161)$$

where Q_s and $\mathcal{M}$ are given, respectively, by Eqs. (15.146) and (15.150).

As long as the matrix $\mathbf{K}$ is positive definite, there are no scalar ghosts. The positivity of $\mathbf{K}$ translates to the conditions that the determinants of principal submatrices of $\mathbf{K}$ are positive, i.e., $K_{11} > 0$ and $Q_s K_{22} > 0$. Provided that $K_{22} > 0$, these conditions are satisfied for

$$Q_s > 0. \quad (15.162)$$

In the small-scale limit, the dispersion relation (12.70) holds in Fourier space. The scalar propagation speed c_s , which is defined by $\omega^2 = c_s^2 k^2/a^2$, obeys

$$(c_s^2 K_{11} - G_{11})(c_s^2 K_{22} - G_{22}) - (c_s^2 K_{12} - G_{12})^2 = 0. \quad (15.163)$$

Let us first consider Horndeski theories in which two particular relations (15.61) are present. On using these relations, we find that the quantity $\mathcal{L}_{,S} = -A_4 - 3HA_5$ is

equivalent to $\mathcal{D} + \mathcal{E} = B_4 + B_{4,N} - HB_{5,N}/2$, i.e.,

$$\mathcal{L}_{,S} = \mathcal{D} + \mathcal{E} \quad (\text{for Horndeski theories}). \quad (15.164)$$

In this case the quantity $\mathcal{M}$ defined by Eq. (15.150) reduces to $\mathcal{M} = 4\mathcal{L}_{,S}^2/\mathcal{W}$, so the propagation speed c_{sH} satisfies

$$c_{sH}^2 K_{12} - G_{12} = -\frac{4\mathcal{L}_{,S}\dot{\chi}}{M_{\text{pl}}\mathcal{W}} (c_{sH}^2 K_{22} - G_{22}). \quad (15.165)$$

Substituting Eq. (15.165) into Eq. (15.163), we obtain two solutions

$$\begin{aligned} c_H^2 &= \frac{G_{11} - [4\mathcal{L}_{,S}\dot{\chi}/(M_{\text{pl}}\mathcal{W})]^2 G_{22}}{K_{11} - [4\mathcal{L}_{,S}\dot{\chi}/(M_{\text{pl}}\mathcal{W})]^2 K_{22}} \\ &= \frac{1}{Q_s} \left[2(\dot{\mathcal{M}} + H\mathcal{M} - \mathcal{E}) - 8 \left(\frac{\mathcal{L}_{,S}\dot{\chi}}{\mathcal{W}} \right)^2 P_{,Y} \right], \end{aligned} \quad (15.166)$$

$$c_m^2 = \frac{G_{22}}{K_{22}} = \frac{P_{,Y}}{P_{,Y} + \dot{\chi}^2 P_{,YY}}. \quad (15.167)$$

The scalar sound speed squared c_H^2 is affected by the existence of the matter field χ , which is consistent with Eq. (12.71). Comparing Eqs. (12.57), (12.68), (12.71) with Eqs. (15.155), (15.146), (15.166), respectively, the quantities w_1, w_2, w_3, w_4 introduced in Eqs. (12.32)–(12.35) are related to ADM geometric scalar quantities, as

$$w_1 = 2\mathcal{L}_{,S} = -2(A_4 + 3HA_5), \quad (15.168)$$

$$w_2 = \mathcal{W} = A_{3,N} + 4HA_{4,N} + 6H^2 A_{5,N} - 4HA_4 - 12H^2 A_5, \quad (15.169)$$

$$\begin{aligned} w_3 = \xi &= 18H^2(A_4 + 3HA_5) + 3(A_{2,N} - 6H^2 A_{4,N} - 12H^3 A_{5,N}) \\ &\quad + \frac{3}{2}(A_{2,NN} + 3HA_{3,NN} + 6H^2 A_{4,NN} + 6H^3 A_{5,NN}), \end{aligned} \quad (15.170)$$

$$w_4 = 2\mathcal{E} = 2B_4 + \dot{B}_5. \quad (15.171)$$

In GLPV theories the relation (15.164) does not hold, so the two propagation speed squares are mixed each other [11, 30]. To quantify the deviation from Horndeski theories, we introduce the parameter

$$\alpha_H \equiv \frac{\mathcal{D} + \mathcal{E}}{\mathcal{L}_{,S}} - 1. \quad (15.172)$$

We also define

$$\beta_H \equiv 2c_m^2 \left(\frac{K_{11}}{Q_s} - 1 \right) \alpha_H = \frac{16\mathcal{L}_{,S}^2(\rho + P)}{\mathcal{W}^2 Q_s} \alpha_H. \quad (15.173)$$

Eliminating the terms G_{22} , G_{11} , G_{12} , and K_{11} in Eq. (15.163) with the help of Eqs. (15.166), (15.167), (15.173) and the relation $G_{12}/K_{12} = (1 + \alpha_H)G_{22}/K_{22}$, the two solutions to Eq. (15.163) are given by [31]

$$c_s^2 = \frac{1}{2} \left[c_m^2 + c_H^2 - \beta_H - \sqrt{(c_m^2 - c_H^2 + \beta_H)^2 + 2c_m^2 \alpha_H \beta_H} \right], \quad (15.174)$$

$$\tilde{c}_m^2 = \frac{1}{2} \left[c_m^2 + c_H^2 - \beta_H + \sqrt{(c_m^2 - c_H^2 + \beta_H)^2 + 2c_m^2 \alpha_H \beta_H} \right]. \quad (15.175)$$

For $c_m^2 \neq 0$, assuming that the deviation from Horndeski theories is small such that $|\alpha_H| \ll 1$, Eqs. (15.174) and (15.175) reduce, respectively, to

$$c_s^2 \simeq c_H^2 - \beta_H + \frac{c_m^2}{2(c_H^2 - c_m^2 - \beta_H)} \alpha_H \beta_H, \quad (15.176)$$

$$\tilde{c}_m^2 \simeq c_m^2 - \frac{c_m^2}{2(c_H^2 - c_m^2 - \beta_H)} \alpha_H \beta_H. \quad (15.177)$$

Even if $|\alpha_H| \ll 1$, this does not necessarily mean that $|\beta_H|$ is also much smaller than 1. The sound speed squared c_s^2 is subject to the modification arising from the deviation from Horndeski theories, such that $c_s^2 \simeq c_H^2 - \beta_H$. On the other hand, provided $|\alpha_H \beta_H| \ll 1$, the correction to the matter sound speed squared c_m^2 is small, such that $\tilde{c}_m^2 \simeq c_m^2$. For non-relativistic matter satisfying $c_m^2 = 0$, the two relations $c_s^2 = c_H^2 - \beta_H$ and $\tilde{c}_m^2 = 0$ exactly hold. Generally, the effect beyond Horndeski theories arises for the scalar sound speed c_s rather than the matter sound speed $\tilde{c}_m$.

For concreteness, let us consider the covariant Galileon and its GLPV extension. The functions $G_{2,3,4,5}$ of covariant Galileons are given by Eq. (12.135), in which case the auxiliary functions F_3 and F_5 can be chosen as $F_3 = c_3 X/(3M^3)$ and $F_5 = 12c_5 X^2/(5M^9)$, respectively. Using the correspondence (15.60), the covariant Galileon corresponds to the functions

$$\begin{aligned} A_2 &= -c_2 X, & A_3 &= \frac{c_3}{3M^3} (2X)^{3/2}, & A_4 &= -\frac{M_{\text{pl}}^2}{2} - \frac{3c_4}{M^6} X^2, \\ A_5 &= \frac{c_5}{2M^9} (2X)^{5/2}, & B_4 &= \frac{M_{\text{pl}}^2}{2} - \frac{c_4}{M^6} X^2, & B_5 &= -\frac{3c_5}{5M^9} (2X)^{5/2}. \end{aligned} \quad (15.178)$$

We recall that the covariant Galileon was constructed to keep the equations of motion up to second order in curved spacetime by adding gravitational counter terms to the covariantized version of the Minkowski Galileon in which partial derivatives of the field are replaced with covariant derivatives. This covariantized Galileon belongs to a class of GLPV theories in which the background and perturbation equations of motion on the flat FLRW background remain of second order. Taking into account the Einstein–Hilbert term $(M_{\text{pl}}^2/2)R$, the Lagrangian of the

covariantized Galileon is given by

$$\begin{aligned} A_2 &= -c_2 X, & A_3 &= \frac{c_3}{3M^3} (2X)^{3/2}, & A_4 &= -\frac{M_{\text{pl}}^2}{2} - \frac{3c_4}{M^6} X^2, \\ A_5 &= \frac{c_5}{2M^9} (2X)^{5/2}, & B_4 &= \frac{M_{\text{pl}}^2}{2}, & B_5 &= 0. \end{aligned} \quad (15.179)$$

The terms $-c_4 X^2/M^6$ and $-3c_5(2X)^{5/2}/(5M^9)$ in B_4 and B_5 of the covariant Galileon Lagrangian (15.178) correspond to the gravitational counter terms eliminating derivatives higher than second order in curved spacetime.

Since the functions $A_{2,3,4,5}$ of covariant Galileons are the same as those of covariantized Galileons, the two theories cannot be distinguished from each other at the background level. However, their difference arises at the level of linear perturbations. In Eq. (12.148) we showed that the sound speed squared for the late-time tracking solution of covariant Galileons is given by $c_s^2 \simeq 1/40$ during the matter-dominated epoch. In the regime $r_1 \ll 1$ and $r_2 \ll 1$, the quantities c_H^2 and β_H of covariantized Galileons during the matter era can be estimated as $c_H^2 \simeq 11/40$ and $\beta_H \simeq -3/10$, respectively, so that $c_s^2 = c_H^2 - \beta_H \simeq -1/40$ [26]. Hence the late-time tracking solution of covariantized Galileons is excluded by the small-scale Laplacian instability. Thus the sound speed squared is a key quantity to distinguish between GLPV theories and Horndeski theories.

15.5. Application to Hořava–Lifshitz gravity

Since our general EFT formalism can encompass theories with spatial derivatives higher than second order, we derive no-ghost and stability conditions in both projectable and non-projectable versions of Hořava–Lifshitz gravity.

15.5.1. Projectable Hořava–Lifshitz gravity

In the original version of Hořava–Lifshitz gravity [15], the lapse N depends on t alone, so the terms α_i ($i = 1, 2, \dots, 5$) vanish. Hence the corresponding action in the presence of a perfect fluid with the k-essence Lagrangian $P(Y)$ is given by

$$S = \int d^4x \sqrt{-g} [\mathcal{L}(K, \mathcal{S}, \mathcal{R}, \mathcal{Z}, \mathcal{Z}_1, \mathcal{Z}_2) + P(Y)], \quad (15.180)$$

where

$$\mathcal{L} = \frac{M_{\text{pl}}^2}{2} [\mathcal{S} - \lambda K^2 + \mathcal{R} - M_{\text{pl}}^{-2} (g_2 \mathcal{R}^2 + g_3 \mathcal{Z}) - M_{\text{pl}}^{-4} (g_4 \mathcal{Z}_1 + g_5 \mathcal{Z}_2)]. \quad (15.181)$$

Since $\delta N = 0$ in the present case, we cannot vary the action (15.180) with respect to δN . Varying (15.180) with respect to $\delta\sqrt{q}$, we obtain Eq. (15.106) with

$$\bar{\mathcal{L}} = 3M_{\text{pl}}^2(1 - 3\lambda)H^2/2, \mathcal{F} = M_{\text{pl}}^2(1 - 3\lambda)H, \text{ i.e.,}$$

$$\frac{3\lambda - 1}{2}M_{\text{pl}}^2(2\dot{H} + 3H^2) = -P. \quad (15.182)$$

The matter field χ obeys Eq. (15.107), which translates to the continuity equation

$$P = -\frac{1}{3a^3H} \frac{d}{dt}(a^3\rho). \quad (15.183)$$

Substituting Eq. (15.183) into Eq. (15.182) and integrating it with respect to t , it follows that

$$\frac{3}{2}(3\lambda - 1)M_{\text{pl}}^2H^2 = \rho + \frac{C}{a^3}, \quad (15.184)$$

where C is an integration constant. The extra term C/a^3 behaves as non-relativistic dark matter [32], which arises due to the absence of the Hamiltonian constraint (see also Refs. [33–35]).

We proceed to the discussion of cosmological perturbations in the absence of the perfect fluid. Since $\delta N = 0$, the perturbation equation (15.128) corresponding the Hamiltonian constraint does not exist. Since $\mathcal{A} = -\lambda M_{\text{pl}}^2$, $\mathcal{L}_{,\mathcal{S}} = M_{\text{pl}}^2/2$, $\mathcal{W} = (3\lambda - 1)M_{\text{pl}}^2H$, and $\mathcal{C} = 0$, the momentum constraint (15.129) leads to

$$\Delta\psi = \frac{3\lambda - 1}{\lambda - 1}\dot{\zeta}, \quad (15.185)$$

which is valid for $\lambda \neq 1$. The quantity $\mathcal{Y}$ defined by Eq. (15.135) yields $\mathcal{Y} = 2M_{\text{pl}}^2(3\lambda - 1)\dot{\zeta}/(\lambda - 1)$. Since $\mathcal{D} = 0$, $\mathcal{E} = M_{\text{pl}}^2/2$, $4\mathcal{G} + 3\mathcal{L}_{,\mathcal{Z}} = -(8g_2 + 3g_3)/2$, and $8\mathcal{L}_{,\mathcal{Z}_1} + 3\mathcal{L}_{,\mathcal{Z}_2} = -(8g_4 + 3g_5)/(2M_{\text{pl}}^2)$, Eq. (15.132) yields [36–38]

$$\frac{d}{dt} \left(\frac{3\lambda - 1}{\lambda - 1} a^3 \dot{\zeta} \right) + a^3 \mathcal{O}\zeta = 0, \quad (15.186)$$

where the operator $\mathcal{O}$ is given by

$$\mathcal{O} \equiv \Delta + \frac{\Delta^2}{M_2^2} - \frac{\Delta^3}{M_3^4}, \quad (15.187)$$

with

$$M_2^2 \equiv M_{\text{pl}}^2(8g_2 + 3g_3)^{-1}, \quad M_3^4 \equiv M_{\text{pl}}^4(8g_4 + 3g_5)^{-1}. \quad (15.188)$$

Substituting $\delta N = 0$ and Eq. (15.185) into the second-order Lagrangian (15.124), it follows that

$$L_2 = M_{\text{pl}}^2 a^3 \left(\frac{3\lambda - 1}{\lambda - 1} \dot{\zeta}^2 - \zeta \mathcal{O}\zeta \right). \quad (15.189)$$

Varying this Lagrangian with respect to ζ , we obtain Eq. (15.186).

For $\lambda \neq 1$, the breaking of gauge symmetry of GR gives rise to the propagation of the scalar degree of freedom ζ . To avoid the appearance of scalar ghosts, we

require that $(3\lambda - 1)/(\lambda - 1) > 0$, i.e., $\lambda > 1$ or $\lambda < 1/3$. At low energy the behavior close to GR should be recovered, so it is natural to consider the regime $\lambda > 1$.

From Eq. (15.189), we obtain the following dispersion relation in the Minkowski spacetime:

$$\omega^2 = \frac{\lambda - 1}{3\lambda - 1} \left(\frac{k^6}{M_3^4} + \frac{k^4}{M_2^2} - k^2 \right). \quad (15.190)$$

For $k \ll \{M_3, M_2\}$, the relation (15.190) reduces to $\omega^2 \simeq -(\lambda - 1)k^2/(3\lambda - 1)$, so the scalar propagation speed squared $c_s^2 = \omega^2/k^2 = -(\lambda - 1)/(3\lambda - 1)$ is negative under the no-ghost condition $(3\lambda - 1)/(\lambda - 1) > 0$. The time scale of this Laplacian instability can be estimated as

$$t_L \approx \frac{1}{k} \sqrt{\frac{3\lambda - 1}{\lambda - 1}}. \quad (15.191)$$

If we consider the evolution of perturbations on the cosmological background, there exists a Hubble friction term $3H\dot{\zeta}(3\lambda - 1)/(\lambda - 1)$ in Eq. (15.186). As long as this term dominates over the Laplacian term $-k^2\zeta$, the instability of scalar perturbations can be avoided for $t_L \gg H^{-1}$. The time scale associated the growth of large-scale structures is given by $t_J \approx M_{\text{pl}}/\sqrt{\rho}$, where ρ is the density of non-relativistic matter. Provided that $t_L \gg t_J$, the structure formation is not affected by the Laplacian instability [39]. In the regime where k is larger than M_3 and M_2 , the first two terms on the right hand side of Eq. (15.190) dominate over $-k^2$, so the Laplacian instability does not arise.

To recover the behavior close to GR at low energy, we require that λ is sufficiently close to 1. Expanding the action (15.180) with (15.181) up to n th order ($n > 2$) in perturbations, the n th order Lagrangian contains the terms with negative powers $(\lambda - 1)^{-(n-1)}$. For larger n the divergence of these terms gets worse for $\lambda \rightarrow 1$, so the perturbative expansion breaks down. This is a strong coupling problem of the projectable version of Hořava–Lifshitz gravity [20, 21].

15.5.2. Non-projectable Hořava–Lifshitz gravity

In the non-projectable Hořava–Lifshitz gravity the lapse N depends on both t and x^i , so the acceleration vector $a_i = \nabla_i \ln N$ does not vanish. In this case the theory is described by the action

$$S = \int d^4x \sqrt{-g} [\mathcal{L}(K, S, \mathcal{R}, \mathcal{Z}, \mathcal{Z}_1, \mathcal{Z}_2, \alpha_1, \dots, \alpha_5) + P(Y)], \quad (15.192)$$

where

$$\begin{aligned} \mathcal{L} = \frac{M_{\text{pl}}^2}{2} [S - \lambda K^2 + \mathcal{R} + \eta_1 \alpha_1 - M_{\text{pl}}^{-2} (g_2 \mathcal{R}^2 + g_3 \mathcal{Z} + \eta_2 \alpha_2 + \eta_3 \alpha_3) \\ - M_{\text{pl}}^{-4} (g_4 \mathcal{Z}_1 + g_5 \mathcal{Z}_2 + \eta_4 \alpha_4 + \eta_5 \alpha_5)]. \end{aligned} \quad (15.193)$$

In the non-projectable Hořava–Lifshitz gravity, there are equations of motion derived by the variation of δN . Let us first discuss the background equations of motion. In the presence of matter with energy density ρ and pressure P , varying the action (15.192) with respect to δN gives rise to Eq. (15.105). This equation translates to

$$\frac{3}{2}(3\lambda - 1)M_{\text{pl}}^2 H^2 = \rho, \quad (15.194)$$

which does not contain the term C/a^3 unlike the projectable case. The momentum constraint and the continuity equation are the same as Eqs. (15.182) and (15.183), respectively.

In the non-projectable Hořava–Lifshitz gravity, it is inconsistent to choose the gauge $\delta N(t, x^i) = 0$ because the gauge transformation (15.71) contains the scalar f depending on t alone. In the following, we proceed to the discussion of cosmological perturbations in the absence of matter without fixing the temporal gauge transformation. Since $\mathcal{W} = (3\lambda - 1)M_{\text{pl}}^2 H$, $\mathcal{L}_{,\alpha_1} = M_{\text{pl}}^2 \eta_1/2$, $\mathcal{L}_{,\alpha_2} = -\eta_2/2$, $\mathcal{L}_{,\alpha_3} = -\eta_3/2$, $\mathcal{L}_{,\alpha_4} = -\eta_4/(2M_{\text{pl}}^2)$, and $\mathcal{L}_{,\alpha_5} = -\eta_5/(2M_{\text{pl}}^2)$, Eqs. (15.128), (15.129), and (15.137) reduce, respectively, to

$$\begin{aligned} & (3\lambda - 1)M_{\text{pl}}^2 H(3\dot{\zeta} - 3H\delta N - \Delta\psi) - 2M_{\text{pl}}^2 \Delta\zeta - M_{\text{pl}}^2 \eta_1 \Delta\delta N + \eta_2 \Delta^2 \delta N \\ & + 2\eta_3 \Delta^2 \zeta + \frac{\eta_4}{M_{\text{pl}}^2} \Delta^3 \delta N + \frac{2\eta_5}{M_{\text{pl}}^2} \Delta^3 \zeta = 0, \end{aligned} \quad (15.195)$$

$$(3\lambda - 1)(\dot{\zeta} - H\delta N) - (\lambda - 1)\Delta\psi = 0, \quad (15.196)$$

$$\Delta(\dot{\psi} + H\psi + \delta N + \zeta) + \frac{\Delta^2 \zeta}{M_2^2} - \frac{\Delta^3 \zeta}{M_3^4} - \frac{\eta_3}{M_{\text{pl}}^2} \Delta^2 \delta N - \frac{\eta_5}{M_{\text{pl}}^4} \Delta^3 \delta N = 0, \quad (15.197)$$

where M_2 and M_3 are defined by Eq. (15.188).

We discuss the stability of perturbations on the Minkowski background ($H = 0$). In the infra-red regime, spatial derivatives higher than second order can be neglected in the perturbation equations of motion. From Eqs. (15.195) and (15.196), we obtain

$$\delta N = -\frac{2}{\eta_1}\zeta, \quad \Delta\psi = \frac{3\lambda - 1}{\lambda - 1}\dot{\zeta}. \quad (15.198)$$

Substituting these relations into Eq. (15.197), we find

$$\frac{3\lambda - 1}{\lambda - 1}\ddot{\zeta} - \frac{2 - \eta_1}{\eta_1}\Delta\zeta = 0. \quad (15.199)$$

The corresponding Lagrangian can be derived by substituting Eq. (15.198) into (15.124) as

$$L_2 = M_{\text{pl}}^2 \frac{3\lambda - 1}{\lambda - 1} \left[\dot{\zeta}^2 - c_s^2 (\partial\zeta)^2 \right], \quad (15.200)$$

where

$$c_s^2 = \frac{\lambda - 1}{3\lambda - 1} \frac{2 - \eta_1}{\eta_1}. \quad (15.201)$$

The parameter space in which both the ghost and the Laplacian instability are absent is given by

$$\frac{3\lambda - 1}{\lambda - 1} > 0, \quad 0 < \eta_1 < 2. \quad (15.202)$$

Thus the coupling η_1 allows the existence of theoretically consistent parameter space. In addition, the strong-coupling problem in the original Hořava–Lifshitz gravity can be alleviated by non-vanishing acceleration terms [22, 25].

To discuss the cosmology after the onset of the radiation era, we need to add the contribution of matter perturbations to Eqs. (15.195)–(15.197). Although the temporal gauge transformation is not fixed, it is possible to study the evolution of cosmological perturbations by considering some gauge-invariant variables like $\zeta_g \equiv \zeta - H\delta\rho/\rho$ [23]. To realize the late-time cosmic acceleration, it is also required to take into account additional source for dark energy to the action of Hořava–Lifshitz gravity. Although the aim of Hořava–Lifshitz gravity is not to modify gravity on infra-red scales associated with the late-time cosmic acceleration, it allows the possibility for studying how the existence of spatial derivatives higher than second order affects observables related to cosmological perturbations.

15.6. Mapping to the EFTCAMB language

After several initial works of the EFT of dark energy [1–4, 6], a numerical code called EFTCAMB was developed for confronting dark energy models with observations [40, 41]. The EFT action used by developers of the EFTCAMB is given by [42]

$$\begin{aligned} S = \int d^4x \sqrt{-g} & \left[\frac{m_0^2}{2} f_*(t) R + \Lambda(t) - c(t) \delta g^{00} + \frac{M_2^4(t)}{2} (\delta g^{00})^2 - \frac{\bar{M}_1^3(t)}{2} \delta g^{00} \delta K \right. \\ & - \frac{\bar{M}_2^2(t)}{2} (\delta K)^2 - \frac{\bar{M}_3^2(t)}{2} \delta K_\nu^\mu \delta K_\mu^\nu + \frac{\hat{M}^2(t)}{2} \delta g^{00} \delta_1 \mathcal{R} + \frac{\bar{m}_5(t)}{2} \delta_1 \mathcal{R} \delta K \\ & + m_2^2(t) \nabla^\mu g^{00} \nabla_\mu g^{00} + \lambda_1(t) (\delta_1 \mathcal{R})^2 + \lambda_2(t) \delta \mathcal{R}_\mu^\nu \delta \mathcal{R}_\nu^\mu + \lambda_3(t) \delta_1 \mathcal{R} \Delta g^{00} \\ & + \lambda_4(t) \nabla^\mu g^{00} (\Delta \nabla_\mu g^{00}) + \lambda_5(t) \nabla^\mu \delta_1 \mathcal{R} \nabla_\mu \delta_1 \mathcal{R} + \lambda_6(t) \nabla^\mu \mathcal{R}_{ij} \nabla_\mu \mathcal{R}_{ij} \\ & \left. + \lambda_7(t) \nabla^\mu g^{00} (\Delta^2 \nabla_\mu g^{00}) + \lambda_8(t) \Delta \mathcal{R} \Delta g^{00} \right] + \int d^4x \sqrt{-g} P(Y), \quad (15.203) \end{aligned}$$

where m_0 is constant, and $f_*, \Lambda, c, M_2^4, \bar{M}_1^3, \bar{M}_2^2, \bar{M}_3^2, \hat{M}^2, \bar{m}_5, m_2^2, \lambda_i$ (with $i = 1, \dots, 8$) are free functions of time (called “EFT functions”). The three functions f_*, Λ, c are associated with background quantities, whereas other EFT functions arise only at the perturbative level. In Ref. [42], the notation $f_*(t) = 1 + \Omega(t)$ was

used, but we adopt $f_*(t)$ for simplicity. Note that we have included the perfect fluid with the k-essence Lagrangian $P(Y)$. In the following, we will relate the time-dependent functions in Eq. (15.203) with those appearing in our general approach including both GLPV theories and Hořava–Lifshitz gravity.

On using the relation (15.33), the four-dimensional Ricci scalar R can be expressed in terms of the three-dimensional quantities. Up to boundary terms, the first term in Eq. (15.203) reads

$$\frac{m_0^2}{2} f_* R = \frac{m_0^2}{2} \left(f_* \mathcal{R} + f_* \mathcal{S} - f_* K^2 - 2 f_* \frac{K}{N} \right). \quad (15.204)$$

We substitute the relations $\mathcal{R} = \delta_1 \mathcal{R} + \delta_2 \mathcal{R}$, $K = 3H^2 + \delta K$, and $\mathcal{S} = 3H^2 + 2H\delta K + \delta K_\nu^\mu \delta K_\mu^\nu$ into Eq. (15.204) and then expand the action (15.203) up to quadratic order in the perturbations. In doing so, we use the fact that the perturbation of $g^{00} = -1/N^2$ is given by $\delta g^{00} = 2\delta N - 3(\delta N)^2$. We also employ the property similar to Eq. (15.95), i.e., $\int d^4x \sqrt{-g} \beta(t) \delta K = \int d^4x \sqrt{-g} (-\dot{\beta} - 3H\beta + \dot{\beta} \delta N - \dot{\beta} \delta N^2)$, where $\beta(t)$ is an arbitrary function of t . Then, the action reduces to the form $S = \int d^4x \sqrt{-g} \mathcal{L}$, with the Lagrangian density

$$\begin{aligned} \mathcal{L} = & m_0^2 (\ddot{f}_* + 2H\dot{f}_* + 2\dot{H}f_* + 3H^2 f_*) + \Lambda + \bar{P} \\ & + [m_0^2 (H\dot{f}_* - 2\dot{H}f_* - \ddot{f}_*) - 2c] \delta N + \frac{m_0^2}{2} f_* \delta_1 \mathcal{R} + P_{,Y} \delta_1 Y \\ & + (m_0^2 \dot{f}_* - \bar{M}_1^3) \delta K \delta N + \frac{1}{2} (m_0^2 f_* - \bar{M}_3^2) \delta K_\nu^\mu \delta K_\mu^\nu - \frac{1}{2} (m_0^2 f_* + \bar{M}_2^2) \delta K^2 \\ & + \hat{M}^2 \delta N \delta \mathcal{R} + \left[m_0^2 (\ddot{f}_* - H\dot{f}_* + 2\dot{H}f_*) + 3c + 2M_2^4 \right] \delta N^2 + \frac{\bar{m}_5}{2} \delta K \delta_1 \mathcal{R} \\ & + 4m_2^2 \nabla_\mu \delta N \nabla^\mu \delta N + \frac{m_0^2}{2} f_* \delta_2 \mathcal{R} + \lambda_1 (\delta_1 \mathcal{R})^2 + \lambda_2 \delta \mathcal{R}_\mu^\nu \delta \mathcal{R}_\nu^\mu + 2\lambda_3 \delta_1 \mathcal{R} \Delta \delta N \\ & + 4\lambda_4 \nabla^\mu \delta N (\Delta \nabla_\mu \delta N) + \lambda_5 \nabla_\mu \delta_1 \mathcal{R} \nabla^\mu \delta_1 \mathcal{R} + \lambda_6 \nabla_\mu \mathcal{R}_{ij} \nabla^\mu \mathcal{R}^{ij} \\ & + 4\lambda_7 \nabla^\mu \delta N (\Delta^2 \nabla_\mu \delta N) + 2\lambda_8 \Delta \delta_1 \mathcal{R} \Delta \delta N + P_{,YY} \delta_2 Y + \frac{P_{,YYY}}{2} \delta_1 Y^2. \end{aligned} \quad (15.205)$$

Comparing terms up to the second line of Eq. (15.205) with those in Eq. (15.109), we find the following correspondence

$$m_0^2 (\ddot{f}_* + 2H\dot{f}_* + 2\dot{H}f_* + 3H^2 f_*) + \Lambda = \bar{\mathcal{L}} - \dot{\mathcal{F}} - 3H\mathcal{F}, \quad (15.206)$$

$$m_0^2 (H\dot{f}_* - 2\dot{H}f_* - \ddot{f}_*) - 2c = \dot{\mathcal{F}} + \mathcal{L}_{,N}, \quad (15.207)$$

$$\frac{m_0^2}{2} f_* = \mathcal{E}. \quad (15.208)$$

The background equations (15.105) and (15.106) can be written as

$$m_0^2(3H^2\dot{f}_* + 3H\dot{f}_*) + \Lambda - 2c = \rho, \quad (15.209)$$

$$m_0^2(\ddot{f}_* + 2H\dot{f}_* + 2\dot{H}f_* + 3H^2f_*) + \Lambda = -P, \quad (15.210)$$

which contain only three EFT parameters f_* , Λ , c . Comparing terms after the third line of Eq. (15.205) with those in Eq. (15.109), it follows that

$$\begin{aligned} M_2^4 &= \frac{1}{4}(2\mathcal{L}_{,N} + \mathcal{L}_{,NN} - 2c), & \bar{M}_2^2 &= -2\mathcal{E} - \mathcal{A}, & \bar{M}_1^3 &= 2\dot{\mathcal{E}} - \mathcal{B}, \\ \bar{M}_3^2 &= 2\mathcal{E} - 2\mathcal{L}_{,S}, & m_2^2 &= \frac{1}{4}\mathcal{L}_{,\alpha_1}, & \bar{m}_5 &= 2\mathcal{C}, & \hat{M}^2 &= \mathcal{D}, \\ \lambda_1 &= \frac{\mathcal{G}}{2}, & \lambda_2 &= \mathcal{L}_{,Z}, & \lambda_3 &= \frac{\mathcal{L}_{,\alpha_3}}{2}, & \lambda_4 &= \frac{\mathcal{L}_{,\alpha_2}}{4}, \\ \lambda_5 &= \mathcal{L}_{,Z_1}, & \lambda_6 &= \mathcal{L}_{,Z_2}, & \lambda_7 &= \frac{\mathcal{L}_{,\alpha_4}}{4}, & \lambda_8 &= \frac{\mathcal{L}_{,\alpha_5}}{2}, \end{aligned} \quad (15.211)$$

where the right hand side can be computed for a given theory.

Let us consider GLPV theories given by the Lagrangian density (15.59) in the ADM language. Computing the terms on the right hand side of Eq. (15.211), it follows that

$$\bar{M}_3^2 = -\bar{M}_2^2, \quad m_2^2 = 0, \quad \bar{m}_5 = 0, \quad \lambda_i = 0, \quad (i = 1, 2, \dots, 8). \quad (15.212)$$

Then, the EFT action (15.203) reduces to

$$\begin{aligned} S &= \int d^4x \sqrt{-g} \left[\frac{m_0^2}{2} f_*(t) R + \Lambda(t) - c(t) \delta g^{00} + \frac{M_2^4(t)}{2} (\delta g^{00})^2 - \frac{\bar{M}_1^3(t)}{2} \delta g^{00} \delta K \right. \\ &\quad \left. - \frac{\bar{M}_2^2(t)}{2} (\delta K^2 - \delta K_\mu^\nu \delta K_\nu^\mu) + \frac{\hat{M}^2(t)}{2} \delta g^{00} \delta_1 \mathcal{R} \right] + \int d^4x \sqrt{-g} P(Y). \end{aligned} \quad (15.213)$$

In this case, there are four EFT functions $M_2^4, \bar{M}_1^3, \bar{M}_2^2, \hat{M}^2$ associated with linear perturbations.

For a given theory whose Lagrangian is written in terms of ADM quantities, the terms on the right hand side of Eq. (15.211) can be explicitly computed. In this case, the time dependence of the EFT functions is known by using the mapping given above. This approach, which is called the *mapping* EFT, allows us to put constraints on a concrete model of the late-time cosmic acceleration from observational data of CMB, LSS, SN Ia, etc. The mapping EFT approach was already used to place bounds on model parameters of $f(R)$ gravity [40].

There is another approach called the *pure* EFT in which the cosmic expansion history is fixed by choosing a particular time dependence of the function $f_*(t)$. The EFT functions $c(t), \Lambda(t)$ are related to $f_*(t)$ according to Eqs. (15.206) and

(15.207). Assuming the time dependence of other EFT functions associated with cosmological perturbations, it is possible to put constraints on their coefficients from observations. The pure EFT approach can be regarded as a model-independent framework to probe the modification of gravity at large distances.

The EFTCAMB code can be downloaded from <http://eftcamb.org>. It remains to be seen whether the signature of modified gravity manifests itself in future high-precision observations.

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Chapter 16

Conclusions

The problem of dark energy has been at the heart of astronomical observations and is driving the way cosmologists and particle physicists are trying to understand the nature of the early and late Universe. In fact, it has led to a remarkable number of publications after its first discovery. More than 4600 papers with the word “dark energy” in the title have appeared on the arXiv between 1998 and 2017, with more than 2300 papers containing “cosmological constant”.

For newcomers to this field, it is not practical to read such huge amount of papers randomly for understanding the essence of dark energy. In this book, I provided fundamentals of the physics of cosmic acceleration by starting from GR. I believe that readers could be able to learn its necessary knowledge and information more efficiently than randomly reading many papers. I also explained basics of other important topics in modern cosmology — such as inflation, cosmological perturbation theory, CMB, and large-scale structures. After readers go through this book, I would suggest them to enter concrete research fields they are interested in. References cited in each chapter will be also useful to find some new research topics.

The research of dark energy is two-fold: (i) one is to constrain models of dark energy from cosmological observations and local gravity experiments, (ii) another is to construct theoretically consistent models of dark energy. Understanding both aspects is essentially important to approach the origin of dark energy, so I provided useful theoretical tools linking theories to observations and experiments.

As for the point (i), I gave a detailed account for the physics of SN Ia, CMB, BAO, galaxy clusterings, weak lensing, and discussed how the properties of dark energy are constrained from those observations. In this book, I did not explain in detail statistical methods employed for placing observational constraints on models. People who are interested in statistical methods in cosmology (like the Monte Carlo method used in CAMB and EFTCAMB) can learn the basics of them in Refs. [1, 2].

Regarding local gravity constraints on dark energy models, I explained two representative screening mechanisms of fifth forces (chameleon and Vainshtein mechanisms) mediated by new propagating degrees of freedom. I applied such mechanisms

to concrete modified gravity models of the late-time cosmic acceleration — such as those based on $f(R)$ gravity, Brans–Dicke theories, Galileons, generalized Proca theories, and identified parameter spaces consistent with solar-system tests of gravity.

As for the point (ii), I explained a broad class of theoretically viable dark energy models proposed in the literature. In particular, I showed that most of single scalar-field models of dark energy belong to a class of most general scalar–tensor theories with second-order equations of motion (Horndeski theories). In the EFT approach of modified gravity, it is also possible to encompass theories with spatial derivatives higher than second order (like those appearing in Hořava–Lifshitz gravity). I provided a general EFT framework encompassing Horndeski theories and its healthy extension (GLPV theories) as well as Hořava–Lifshitz gravity. The background and linear perturbation equations of motion presented in Chap. 15 can be applied to constrain a wide variety of dark energy models by using the correspondence between EFT functions introduced in the EFTCAMB code and the Lagrangian expressed in term of the ADM language.

While Horndeski theories have one scalar propagating degree of freedom (spin 0), there are also dark energy models based on a massive vector field (spin 1) with derivative interactions (generalized Proca theories). In this case, there are two transverse vector polarizations in addition to one scalar mode. Derivative interactions allow the existence of a de Sitter attractor relevant to the late-time acceleration. I derived conditions for the absence of ghosts and Laplacian instabilities on the FLRW background for scalar, vector, tensor perturbations and applied them to a class of dark energy models in the framework of generalized Proca theories. There exists a wide range of the parameter space consistent with the absence of ghosts and Laplacian instabilities. The generalized Proca theories also allow the gravitational interaction weaker than that of GR on scales relevant to large-scale structures.

There are also theories of a massive spin-2 field in which the graviton has a non-vanishing mass. As I mentioned in Sec. 14.2, the original DRGT massive gravity [3], which was constructed to avoid the appearance of the BD ghost in a Lorentz-invariant way, does not allow the existence of stable isotropic and homogeneous cosmological solutions. However, there still remain some possibilities to avoid such problems in several extended versions of DRGT massive gravity [4–6]. A simple extension of the dRGT theory also allows the construction of a fully non-linear bimetric theory of gravity with two metrics [7–9]. There are also Lorentz-violating massive gravity theories without theoretical pathologies [10–12] and non-local formulations of massive gravity [13–15]. I refer the reader to the review article [16] for recent progress of massive gravity and bigravity.

Besides massive gravity, I did not explain details of several modified gravity theories in this book. The reader may have a look at the references [17–19] for the reviews of other modified gravity theories. For example, there are dark energy models based on the Gauss–Bonnet coupling $F(\phi)\mathcal{G}$ [20] with a scalar field ϕ and on the theories with the Lagrangian $f(\mathcal{G})$ (where $\mathcal{G}$ is the Gauss–Bonnet term)

[21]. Both of them belong to sub classes of Horndeski theories [22]. If such terms are relevant to the cosmic acceleration, however, the perturbations are typically subject to the ghost or the Laplacian instabilities [23–26].

In this book, we discussed Hořava–Lifshitz gravity as a Lorentz-violating theory in the ultra-violet regime, but there are also other theories like Einstein–Aether theory with a vector field in a preferred direction [27, 28] and Lorentz-violating vector-field condensates [29, 30]. Especially in the latter Lorentz-violating theory, it is possible to realize an infrared modification of gravity with a phantom equation of state by avoiding pathological behavior of perturbations in the ultraviolet regime [31, 32].

The current observational status of dark energy models is that the cosmological constant is still compatible with the joint data analysis of SN Ia, CMB, and BAO. There has been no strong observational evidence that the dark energy equation of state w_{DE} larger than -1 is favored over the cosmological constant. In particular, the models in which w_{DE} is initially away from -1 and then approaches -1 at late times are disfavored from the data. The models with $w_{\text{DE}} < -1$, which can be realized in modified gravity theories, are consistent with the data, as long as w_{DE} is not significantly away from -1 . There are several theoretical models already excluded from the joint data analysis of SN Ia, CMB, and BAO, such as the freezing quintessence described by the potential $V(\phi) \propto \phi^{-n}$ with $n \geq 1$, the DGP braneworld model, and the tracker solution of covariant Galileons. The void model without the real cosmic acceleration is also in strong tension with the combined data analysis of SN Ia and BAO.

Adding information of the growth history to the background can put further constraints on dark energy models. This is especially the case for modified gravity models in which the effective gravitational coupling G_{eff} with non-relativistic matter is different from the Newton gravitational constant on scales relevant to the large-scale structure formation. In Horndeski theories, we derived a convenient expression of G_{eff} under a quasi-static approximation on sub-horizon scales and applied this general result to concrete modified gravity models like $f(R)$ gravity, Brans–Dicke theories, and covariant Galileons. Due to the presence of an extra interaction between a scalar degree of freedom and matter, G_{eff} is typically larger than G in dark energy models within the framework of Horndeski theories.

From the observational side, the amplitude of matter perturbations (σ_8) constrained from the Planck CMB data [33, 34] has been in tension with that in low-redshift measurements including red-shift space distortions [35–37]. If we use the value of σ_8 constrained from the Planck data, then the growth rate $f\sigma_8$ predicted by the Λ CDM model tends to be larger than their values in the RSD data. This may be attributed to the tension of the Hubble constant between Planck and the direct measurements of H_0 , but it also shows another possibility for the gravitational interaction weaker than that in GR. If the latter is really the case, this provides important information for constraining modified gravity theories.

In Horndeski theories, it is generally difficult to realize $G_{\text{eff}} < G$ unless the tensor sector of theories is substantially modified, but in generalized Proca theories the presence of additional vector degrees of freedom allows the possibility for realizing $G_{\text{eff}} < G$ while avoiding ghosts and instability problems. In current RSD measurements, however, the error bars of $f\sigma_8$ have been still too large to put tight bounds on modified gravity theories. The models in which G_{eff} is significantly larger than G are disfavored from the RSD data, but we cannot clearly distinguish between different modified gravity models from the current RSD data alone. In upcoming observations like EUCLID,¹ it is expected that the growth rate will be constrained more tightly. It remains to be seen whether the tension between CMB and RSD data persists in future observations. Other independent observational data such as those from weak lensing will provide important constraints on dark energy models.

While this book was under the process of final proofreading, there was the news for the detection of gravitational waves from a binary neutron star merger with an electromagnetic counterpart [38]. The speed c_t of gravitational waves traveling over the cosmological distance was constrained to be very close to the speed of light c , as $-3 \times 10^{-15} \leq c_t/c - 1 \leq 7 \times 10^{-16}$. In Horndeski/GLPV theories where the functions G_4 and G_5 contain the dependence of kinetic energy $X = -\nabla_\mu \phi \nabla^\mu \phi / 2$ and in generalized Proca theories with the quartic and quintic interactions, c_t is generally different from 1. Hence such theories can be tightly constrained from the bound of c_t mentioned above. Thus, the discovery of gravitational waves opened up a new avenue for probing the modification of gravity on cosmological scales.

When the cosmic acceleration was first found in 1998, the cosmological constant ($w_{\text{DE}} = -1$) was assumed in the likelihood analysis of SN Ia. This reflected the fact that observational constraints on w_{DE} were weak at that time. Independent observational data from CMB and BAO broke this degeneracy and allowed one to place tighter constraints on w_{DE} . It is expected that new data in future will further improve bounds on w_{DE} . Ultimately we would like to clarify whether the deviation of w_{DE} from -1 can be seen from the data. Especially, if the region $w_{\text{DE}} > -1$ were excluded from observations, this will provide important information for the model building of dark energy.

If we do not see any signature for the deviation of w_{DE} from -1 in future observations, we need to address the cosmological constant problem in such a way that there is a left-over tiny vacuum energy responsible for the current cosmic acceleration. The vacuum energy sequestering discussed in Chap. 9 offers one of such possibilities. If future observational data point to the value w_{DE} smaller than -1 , it can be a signature of modified gravity theories. In this case, the growth data will be crucially important to distinguish between different modified gravity models.

¹See the webpage: <http://sci.esa.int/euclid/>.

Although there are still many stumbling blocks to identify the origin of dark energy completely, I hope that we will be able to do so in future with the development of both theories and observations (at least by the end of this century!).

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Appendix A

Equations of Motion in Horndeski Theories

The action of Horndeski theories is given by Eq. (12.1) with the four Lagrangian densities (12.2)–(12.5). In the presence of matter with the energy-momentum tensor $T_{\mu\nu}$, the gravitational equations and the scalar-field equation are given, respectively, by Eqs. (12.16) and (12.18). The explicit forms of the terms $\mathcal{G}_{\mu\nu}^{(i)}$ (where $i = 2, 3, 4, 5$) in Eq. (12.16) are

$$\mathcal{G}_{\mu\nu}^{(2)} = -G_{2,X} \nabla_\mu \phi \nabla_\nu \phi / 2 - G_2 g_{\mu\nu} / 2, \quad (\text{A.1})$$

$$\mathcal{G}_{\mu\nu}^{(3)} = G_{3,X} \square \phi \nabla_\mu \phi \nabla_\nu \phi / 2 + \nabla_{(\mu} G_3 \nabla_{\nu)} \phi - g_{\mu\nu} \nabla_\lambda G_3 \nabla^\lambda \phi / 2, \quad (\text{A.2})$$

$$\begin{aligned} \mathcal{G}_{\mu\nu}^{(4)} = & G_4 G_{\mu\nu} - G_{4,X} R \nabla_\mu \phi \nabla_\nu \phi / 2 \\ & - G_{4,XX} [(\square \phi)^2 - (\nabla_\alpha \nabla_\beta \phi)(\nabla^\alpha \nabla^\beta \phi)] \nabla_\mu \phi \nabla_\nu \phi / 2 \\ & - G_{4,X} \square \phi \nabla_\mu \nabla_\nu \phi + G_{4,X} \nabla_\lambda \nabla_\mu \phi \nabla^\lambda \nabla_\nu \phi + 2 \nabla_\lambda G_{4,X} \nabla^\lambda \nabla_{(\mu} \phi \nabla_{\nu)} \phi \\ & - \nabla_\lambda G_{4,X} \nabla^\lambda \phi \nabla_\mu \nabla_\nu \phi + g_{\mu\nu} (G_{4,\phi} \square \phi - 2X G_{4,\phi\phi}) \\ & + g_{\mu\nu} \{-2G_{4,\phi X} \nabla_\alpha \nabla_\beta \phi \nabla^\alpha \phi \nabla^\beta \phi + G_{4,XX} \nabla_\alpha \nabla_\lambda \phi \nabla_\beta \nabla^\lambda \phi \nabla^\alpha \phi \nabla^\beta \phi \\ & + G_{4,X} [(\square \phi)^2 - (\nabla_\alpha \nabla_\beta \phi)(\nabla^\alpha \nabla^\beta \phi)] / 2\} + 2[G_{4,X} R_{\lambda(\mu} \nabla_{\nu)} \phi \nabla^\lambda \phi \\ & - \nabla_{(\mu} G_{4,X} \nabla_{\nu)} \phi \square \phi] - g_{\mu\nu} (G_{4,X} R^{\alpha\beta} \nabla_\alpha \phi \nabla_\beta \phi - \nabla_\lambda G_{4,X} \nabla^\lambda \phi \square \phi) \\ & + G_{4,X} R_{\mu\alpha\nu\beta} \nabla^\alpha \phi \nabla^\beta \phi - G_{4,\phi} \nabla_\mu \nabla_\nu \phi - G_{4,\phi\phi} \nabla_\mu \phi \nabla_\nu \phi \\ & + 2G_{4,\phi X} \nabla^\lambda \phi \nabla_\lambda \nabla_{(\mu} \phi \nabla_{\nu)} \phi - G_{4,XX} \nabla^\alpha \phi \nabla_\alpha \nabla_\mu \phi \nabla^\beta \phi \nabla_\beta \nabla_\nu \phi, \end{aligned} \quad (\text{A.3})$$

$$\begin{aligned} \mathcal{G}_{\mu\nu}^{(5)} = & G_{5,X} R_{\alpha\beta} \nabla^\alpha \phi \nabla^\beta \nabla_{(\mu} \phi \nabla_{\nu)} \phi - G_{5,X} R_{\alpha(\mu} \nabla_{\nu)} \phi \nabla^\alpha \phi \square \phi \\ & - G_{5,X} R_{\alpha\beta} \nabla^\alpha \phi \nabla^\beta \phi \nabla_\mu \nabla_\nu \phi / 2 - G_{5,X} R_{\mu\alpha\nu\beta} \nabla^\alpha \phi \nabla^\beta \phi \square \phi / 2 \\ & + G_{5,X} R_{\alpha\lambda\beta(\mu} \nabla_{\nu)} \phi \nabla^\lambda \phi \nabla^\alpha \nabla^\beta \phi + G_{5,X} R_{\alpha\lambda\beta(\mu} \nabla_{\nu)} \nabla^\lambda \phi \nabla^\alpha \phi \nabla^\beta \phi \\ & - \nabla_{(\mu} [G_{5,X} \nabla^\alpha \phi] \nabla_\alpha \nabla_{\nu)} \phi \square \phi / 2 + \nabla_{(\mu} [G_{5,\phi} \nabla_{\nu)} \phi] \square \phi / 2 \\ & - \nabla_\lambda [G_{5,\phi} \nabla_{(\mu} \phi] \nabla_{\nu)} \nabla^\lambda \phi \\ & + [\nabla_\lambda (G_{5,\phi} \nabla^\lambda \phi) - \nabla_\alpha (G_{5,X} \nabla_\beta \phi) \nabla^\alpha \nabla^\beta \phi] \nabla_\mu \nabla_\nu \phi / 2 \\ & + \nabla^\alpha G_5 \nabla^\beta \phi R_{\alpha(\mu\nu)\beta} - \nabla_{(\mu} G_5 G_{\nu)\lambda} \nabla^\lambda \phi \\ & + \nabla_{(\mu} G_{5,X} \nabla_{\nu)} \phi [(\square \phi)^2 - (\nabla_\alpha \nabla_\beta \phi)(\nabla^\alpha \nabla^\beta \phi)] / 2 \\ & - \nabla^\lambda G_5 R_{\lambda(\mu} \nabla_{\nu)} \phi + \nabla_\alpha (G_{5,X} \nabla_\beta \phi) \nabla^\alpha \nabla_{(\mu} \phi \nabla_{\nu)} \nabla^\beta \phi \\ & - \nabla_\beta G_{5,X} [\square \phi \nabla^\beta \nabla_{(\mu} \phi - \nabla^\alpha \nabla^\beta \phi \nabla_\alpha \nabla_{(\mu} \phi] \nabla_{\nu)} \phi \\ & + \nabla^\alpha \phi \nabla_\alpha G_{5,X} (\square \phi \nabla_\mu \nabla_\nu \phi - \nabla_\beta \nabla_\mu \phi \nabla^\beta \nabla_\nu \phi) / 2 \end{aligned}$$

$$\begin{aligned}
& -G_{5,X}G_{\alpha\beta}\nabla^\alpha\nabla^\beta\phi\nabla_\mu\phi\nabla_\nu\phi/2 - G_{5,X}\Box\phi\nabla_\alpha\nabla_\mu\phi\nabla^\alpha\nabla_\nu\phi/2 \\
& + G_{5,X}(\Box\phi)^2\nabla_\mu\nabla_\nu\phi/2 + G_{5,XX}[(\Box\phi)^3 - 3\Box\phi(\nabla_\alpha\nabla_\beta\phi)(\nabla^\alpha\nabla^\beta\phi) \\
& + 2(\nabla^\mu\nabla_\nu\phi)(\nabla^\nu\nabla_\lambda\phi)(\nabla^\lambda\nabla_\mu\phi)]\nabla_\mu\phi\nabla_\nu\phi/12 + \nabla_\lambda G_5 G_{\mu\nu}\nabla^\lambda\phi/2 \\
& + g_{\mu\nu}\left\{-G_{5,X}[(\Box\phi)^3 - 3\Box\phi(\nabla_\alpha\nabla_\beta\phi)(\nabla^\alpha\nabla^\beta\phi) \right. \\
& + 2(\nabla^\mu\nabla_\nu\phi)(\nabla^\nu\nabla_\lambda\phi)(\nabla^\lambda\nabla_\mu\phi)]/6 + \nabla_\alpha G_5 R^{\alpha\beta}\nabla_\beta\phi - \nabla_\alpha(G_{5,\phi}\nabla^\alpha\phi)\Box\phi/2 \\
& + \nabla_\alpha(G_{5,\phi}\nabla_\beta\phi)\nabla^\alpha\nabla^\beta\phi/2 - \nabla_\alpha G_{5,X}\nabla^\alpha X\Box\phi/2 + \nabla_\alpha G_{5,X}\nabla_\beta X\nabla^\alpha\nabla^\beta\phi/2 \\
& - \nabla^\lambda G_{5,X}\nabla_\lambda\phi[(\Box\phi)^2 - (\nabla_\alpha\nabla_\beta\phi)(\nabla^\alpha\nabla^\beta\phi)]/4 \\
& \left. + G_{5,X}R_{\alpha\beta}\nabla^\alpha\phi\nabla^\beta\phi\Box\phi/2 - G_{5,X}R_{\alpha\lambda\beta\rho}\nabla^\alpha\nabla^\beta\phi\nabla^\lambda\phi\nabla^\rho\phi/2\right\}, \tag{A.4}
\end{aligned}$$

where we used the notation

$$A^{(\mu_1\cdots\mu_n)} = \frac{1}{n!} \sum_{\text{permutation}} A^{\mu_1\cdots\mu_n}, \tag{A.5}$$

for the symmetrization of a n -rank tensor $A^{\mu_1\cdots\mu_n}$.

The terms $P_\phi^{(i)}$ and $J_\phi^{(i)}$ (where $i = 2, 3, 4, 5$) in Eq. (12.18) are given, respectively by

$$P_\phi^{(2)} = G_{2,\phi}, \tag{A.6}$$

$$P_\phi^{(3)} = \nabla_\mu G_{3,\phi}\nabla^\mu\phi, \tag{A.7}$$

$$P_\phi^{(4)} = G_{4,\phi}R + G_{4,\phi X}[(\Box\phi)^2 - (\nabla_\mu\nabla_\nu\phi)(\nabla^\mu\nabla^\nu\phi)], \tag{A.8}$$

$$\begin{aligned}
P_\phi^{(5)} = & -\nabla_\mu G_{5,\phi}G^{\mu\nu}\nabla_\nu\phi - G_{5,\phi X}[(\Box\phi)^3 - 3\Box\phi(\nabla_\mu\nabla_\nu\phi)(\nabla^\mu\nabla^\nu\phi) \\
& + 2(\nabla^\mu\nabla_\nu\phi)(\nabla^\nu\nabla_\lambda\phi)(\nabla^\lambda\nabla_\mu\phi)]/6, \tag{A.9}
\end{aligned}$$

and

$$J_\mu^{(2)} = -\mathcal{L}_{2,X}\nabla_\mu\phi, \tag{A.10}$$

$$J_\mu^{(3)} = -\mathcal{L}_{3,X}\nabla_\mu\phi + G_{3,X}\nabla_\mu X + 2G_{3,\phi}\nabla_\mu\phi, \tag{A.11}$$

$$\begin{aligned}
J_\mu^{(4)} = & -\mathcal{L}_{4,X}\nabla_\mu\phi + 2G_{4,X}R_{\mu\nu}\nabla^\nu\phi - 2G_{4,XX}(\Box\phi\nabla_\mu X - \nabla^\nu X\nabla_\mu\nabla_\nu\phi) \\
& - 2G_{4,\phi X}(\Box\phi\nabla_\mu\phi + \nabla_\mu X), \tag{A.12}
\end{aligned}$$

$$\begin{aligned}
J_\mu^{(5)} = & -\mathcal{L}_{5,X}\nabla_\mu\phi - 2G_{5,\phi}G_{\mu\nu}\nabla^\nu\phi \\
& - G_{5,X}(G_{\mu\nu}\nabla^\nu X + R_{\mu\nu}\Box\phi\nabla^\nu\phi - R_{\nu\lambda}\nabla^\nu\phi\nabla^\lambda\nabla_\mu\phi - R_{\alpha\mu\beta\nu}\nabla^\nu\phi\nabla^\alpha\nabla^\beta\phi) \\
& + G_{5,XX}\left\{\nabla_\mu X[(\Box\phi)^2 - (\nabla_\alpha\nabla_\beta\phi)(\nabla^\alpha\nabla^\beta\phi)]/2 \right. \\
& \left. - \nabla_\nu X(\Box\phi\nabla_\mu\nabla^\nu\phi - \nabla_\alpha\nabla_\mu\phi\nabla^\alpha\nabla^\nu\phi)\right\} \\
& + G_{5,\phi X}\left\{\nabla_\mu\phi[(\Box\phi)^2 - (\nabla_\alpha\nabla_\beta\phi)(\nabla^\alpha\nabla^\beta\phi)]/2 \right. \\
& \left. + \Box\phi\nabla_\mu X - \nabla^\nu X\nabla_\nu\nabla_\mu\phi\right\}. \tag{A.13}
\end{aligned}$$

Appendix B

Effective Mass Term in Horndeski Theories

The term M_ϕ^2 defined by Eq. (12.41), which appears in the linear perturbation equations of motion in Horndeski theories, is related to the mass squared of the scalar degree of freedom. The explicit form of M_ϕ^2 is given by

$$\begin{aligned}
M_\phi^2 = & -G_{2,\phi\phi} + (\ddot{\phi} + 3H\dot{\phi})G_{2,\phi X} + 2XG_{2,\phi\phi X} + 2X\ddot{\phi}G_{2,\phi XX} \\
& + [6H(G_{3,\phi XX}X + G_{3,\phi X})\dot{\phi} - 2G_{3,\phi\phi X}X - 2G_{3,\phi\phi}]\ddot{\phi} \\
& + 6H(G_{3,\phi\phi X}X - G_{3,\phi\phi})\dot{\phi} + 6G_{3,\phi X}X\dot{H} + 2(9H^2G_{3,\phi X} - G_{3,\phi\phi\phi})X \\
& + [6H^2(4G_{4,\phi XXX}X^2 + 8G_{4,\phi XX}X + G_{4,\phi X}) \\
& - 6H(2G_{4,\phi\phi XX}X + 3G_{4,\phi\phi X})\dot{\phi}] \ddot{\phi} + [12H(G_{4,\phi X} + 2G_{4,\phi XX}X)\dot{H} \\
& + 6H(6H^2G_{4,\phi XX}X - 2G_{4,\phi\phi\phi X}X + 3H^2G_{4,\phi X})]\dot{\phi} \\
& + 12H^2(2G_{4,\phi\phi XX}X^2 - 3G_{4,\phi\phi X}X - G_{4,\phi\phi}) - 6(2G_{4,\phi\phi X}X + G_{4,\phi\phi})\dot{H} \\
& + [2H^3(2G_{5,\phi XXX}X^2 + 7G_{5,\phi XX}X + 3G_{5,\phi X})\dot{\phi} \\
& - 6H^2(5G_{5,\phi\phi X}X + G_{5,\phi\phi} + 2G_{5,\phi\phi XX}X^2)] \ddot{\phi} \\
& + [2H^3(2G_{5,\phi\phi XX}X^2 - 9G_{5,\phi\phi} - 7G_{5,\phi\phi X}X) - 12H(G_{5,\phi\phi X}X + G_{5,\phi\phi})\dot{H}]\dot{\phi} \\
& + 6H^2X(3H^2G_{5,\phi X} - G_{5,\phi\phi\phi} + 2H^2G_{5,\phi XX}X - 2G_{5,\phi\phi\phi X}X) \\
& + 6H^2X(3G_{5,\phi X} + 2G_{5,\phi XX}X)\dot{H}.
\end{aligned} \tag{B.1}$$

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Preface

With the increasing data from the sky, it becomes clear now that matter in the Universe is dominated by dark matter (DM). However, there is no hint that some elementary or composite particle in particle physics is identifiable as DM.

This book is not a topical review article for physicists working in this field, but is an introductory textbook on dark matter for senior graduate students. At this interim level, I try to include many relevant references at the end of each chapter.

As a textbook, we emphasize the symmetry principle of quantum mechanics (QM) as the theoretical basis for DM. In the second half of the 20th century, quantum field theory — the cherished son of QM — evolved to the standard model (SM) in particle physics. At present, especially after the discovery of the Brout–Englert–Higgs–Guralnik–Hagen–Kibble boson (abbreviated as “Higgs boson” in this book), there is no major convincing evidence against the SM even from the 13 TeV high-energy data of Large Hadron Collider (LHC) at CERN. The SM is a gauge theory with gauge group $SU(3) \times SU(2) \times U(1)$. There are twelve spin 1 gauge bosons: the strongly interacting eight gluons, and $W_\mu^\pm$, Z_μ^0 , and photon. The matter fields of the SM are commonly considered as 49, which counts three families of spin $\frac{1}{2}$ fermions and the spin 0 Higgs boson. Out of the 49 matter fields, 46 are lighter than 200 GeV. The remaining three are the so-called singlet (or right-handed) neutrinos. One may exclude these three from the SM spectrum. The observed neutrino oscillation phenomena, however, require the singlet neutrinos in the SM spectrum. At present, it is not known the mass scale of these singlet neutrinos. Depending on its mass scale, in principle one of them can be a candidate of DM particles.

However, the most probable DM particle candidates seem to be some particle(s) beyond the standard model (BSM). Therefore, the main journey of this book is on the candidate DM particles in the BSM. Disregarding the neutrino mixing parameters, the number of parameters in the SM is 19. Out of these, two hierarchy parameters are the QCD vacuum angle $\bar{\theta}$ and the Higgs mass parameter $-\mu^2$. Since 1980s, the BSM physics has evolved to understand these hierarchy parameters. Most efforts to introduce DM particles are also connected to these hierarchy problems. At

the field theory level, it is fair to say that the hierarchy problem is not as desperate as the nonrenormalizability problem present in the old V–A theory of weak interactions on the road to the SM. Some BSMs such as technicolor were easily ruled out by precision experiments. Even supersymmetry (SUSY) the front runner among the hierarchy solutions, having been around for almost four decades, is not confirmed by the LHC experiments. Fortunately, DM discussions do not directly depend on the ideas related to hierarchy problems.

In the sky, there seems to be nonluminous extra matter which is called dark matter. Existence of DM was proposed more than eight decades ago by F. Zwicky by studying motion of galaxies in the Coma Cluster. Since 1970s after accurately measuring rotation velocities of stars in the clusters of galaxies, existence of DM has been widely accepted. Recent observations of the gravitational lensing effects also suggest the existence of DM. However, there is no hint on the nature of DM.

If DM exists, it must be some kind of particle without the ability of shining in the sky; its interaction must be weaker than the electromagnetic interaction. But to fit the astrophysical observation related to DM, its interaction must be much weaker than the electromagnetic interaction. In addition, it is present in the sky now, i.e., it is absolutely stable or unstable with lifetime greater than 10^{26} s. With this observation, the hypothesis on the existence of DM is pursued theoretically based on symmetry principles. Two symmetry principles (continuous and discrete symmetries) give two classes of DM as the BSM particles. One class is based on some global symmetry in which the bosonic collective motion (BCM) is working as DM. The ingredient of BCM is some boson, and they move almost in the same way in the collective motion. The mass of this boson is very light. The other class is based on some discrete symmetry in which some massive particle is weakly interacting without shining in the sky, leading to the name weakly interacting massive particle (WIMP). A WIMP can be boson or fermion.

There can be many BCM possibilities for DM among which the QCD axion is the front runner. The so-called “invisible” axion DM in the Universe is a QCD axion. The window of its decay constant is $10^9 \text{ GeV} \lesssim f_a \lesssim 10^{11} \text{ GeV}$. Its lifetime is more than 10^{40} years, and the number density around Sun is 10^{13} cm^{-3} . “Axion” is a word related to an “axial” current in the days of “PCAC”. An axial current of Dirac fermion field ψ is $j^\mu = \bar{\psi}\gamma^\mu\gamma_5\psi$. “PCAC” means that the Axial Current is not exactly conserved but only Partially Conserved, implying the appearance of a massive pseudoscalar boson. In the modern terminology, it can be said that “axion” is a pseudo-Goldstone boson corresponding to spontaneous breaking of a “global U(1) axial symmetry”. The QCD axion means that the U(1) symmetry is exactly conserved except for the QCD anomaly. This U(1) symmetry possessing the QCD anomaly is called the Peccei–Quinn U(1) global symmetry.

WIMPs must be absolutely stable or close to that if unstable, with lifetime greater than 10^{26} s. The stability of a WIMP can be assured if the SM particles and the WIMP belong to different classes such that one WIMP cannot decay only to SM

particles. The discrete quantum numbers are the well-known strategy for assigning different quantum numbers to the WIMP and the SM particles. Among numerous WIMP possibilities, the so-called lightest supersymmetric particle (LSP) in the supersymmetric extension of the SM is most well known. The discrete symmetry in this case is R -parity, and the LSP carries R -parity -1 while the SM particles carry R -parity $+1$. Dark matter WIMP is a special case of massive DM particles. Stable massive particles can be a consequence of an exact global symmetry also as a proton is stable under the assumption of conserved baryon number based on the exact global symmetry $U(1)_B$. Thus, massive DM particles may be a consequence of a global symmetry $U(1)_{\text{dark matter}}$, whose mechanism is called asymmetric DM. In this case, creation of global quantum numbers must follow Sakharov's three conditions on the creation of global quantum numbers in the Universe.

So, the symmetry principle is the key word in particle physics and DM in the Universe. We try to introduce each concept precisely and then present its physical and cosmological implications colloquially.

Jihn E. Kim
January, 2017

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Symbol	Name, equation	Value
$g_{\mu\nu}$	spacetime metric tensor	$\eta_{\mu\nu} = \text{diag.}(-1, +1, +1, \dots, +1)$
c	speed of light = 1	299,792,458 m/s
$\hbar$	Planck constant = 1	$1.054571726(47) \times 10^{-34}$ J s
	GeV · s	1.519255×10^{24}
	GeV · cm	0.5067689×10^{14}
	GHz	4.136×10^{-6} eV
	°K	0.861735×10^{-4} eV
H_0	Hubble constant ($\sqrt{\rho/3M_P^2}$)	$h \times 10^{-42}$ GeV ($h \simeq 0.674$)
t	cosmic time in radiation-dominated phase	$\sim (10^{-3} \text{ GeV}/T)^2 \text{ s}$
t_U	current age	$\approx 4.3 \times 10^{17}$ s
	pc	$3.09 \times 10^{18} \text{ cm} = 3.26 \text{ light years}$
$R(t), a(t)$	scale factor	$4 \times 10^3 \text{ Mpc at } t = t_U$
ρ_c	critical density today ($0.81h^2 \times 10^{-46} \text{ GeV}^4$)	$1.88h^2 \times 10^{-29} \text{ g cm}^{-3} \text{ at } t = t_U$
Ω_b	baryon fraction today	~ 0.05
Ω_{CDM}	CDM fraction today	~ 0.27
Ω_Λ	dark energy fraction today	~ 0.68
σ_8	RMS matter fluctuation size today in linear theory	~ 0.83
τ	Thomson scattering optical depth due to reionization	0.01–0.8
n_s	scalar spectrum power-law index	$\sim 0.97 \text{ at } k_0 = 0.05 \text{ Mpc}^{-1}$
n_t	tensor spectrum power-law index	$-r_{0.05}/8$
A_s	dimensionless curvature power spectrum	given at $k_0 = 0.05 \text{ Mpc}^{-1}$
θ_{MC}	approximation to r_*/D_Λ	$\sim 0.005\text{--}0.1$
z_{re}	redshift at which Universe is half reionized	~ 11.4
T_D	temperature at the time of X decay	
T_{dec}	decoupling temperature of DM	
T_{fr}	freeze-out temperature of DM	
M_P	reduced Planck mass = $(8\pi G_N)^{-1/2}$	$2.436 \times 10^{18} \text{ GeV}$
M_{GUT}	grand unification scale $\simeq M_U$ definition	$\sim (2\text{--}3) \times 10^{16} \text{ GeV}$
v_{ew}	electroweak symmetry breaking scale	246 GeV
G_F	Fermi coupling constant	$1.16639 \times 10^{-5} \text{ GeV}^{-2}$
$\sin^2 \theta_W$	weak mixing angle	0.23113(15)
M_Z	Z boson mass = $\frac{1}{2} g v_{\text{ew}} \sec \theta_W$	91.1876(21) GeV
M_S	scale for SUSY breaking source	unknown
M_{SUSY}	observable sector SUSY splitting scale	unknown
$\mathbf{Z}_N$	discrete symmetry of order N	
ϑ	anticommuting variable in SUSY	
$\bar{\theta}$	low energy QCD vacuum angle	
a	axion	
$\tilde{a}$	axino	
$\tilde{G}$	gravitino	
χ	X neutralino	

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Chapter 1

Introduction

*Scientific views end in awe and mystery, lost at
the edge in uncertainty — R. Feynman*

1.1. Astroparticle physics and cosmic energy pie

Eighty odd years have elapsed since Zwicky [1] speculated the existence of a large amount of nonluminous (dark) matter to account for gravitational binding of the constituent galaxies of the Coma Cluster. Since that time, the puzzle of exactly what constitutes the dark matter (DM), by which elementary particles, has become one of the foremost unresolved questions in particle physics and cosmology, in the realm of the so-called astroparticle physics. To probe the Universe and stellar objects, astroparticle physics uses all the cosmic ray (CR) particles of the standard model (SM), while astrophysics uses only the CR electromagnetic waves. This is the difference in the words between “astroparticle physics” and “astrophysics”.

All particles of the SM have been discovered, with the last one the Brout–Englert–Higgs–Guralnik–Hagen–Kibble (BEHGHK) boson h of mass 125 GeV discovered at the Large Hadron Collider (LHC) of CERN.¹ The SM particles are shown in the cartoon Fig. 1.1, where the strongly interacting particles are colored. The “color” cannot be seen at low energy due to the color (or quark) confinement. Because the SM has been almost confirmed below the TeV energy scale, it is reliable to look at our Universe for CRs up to 10^{21} eV without much uncertainty from particle physics theory, but the Greisen–Kuz’mín–Zatsepin (GZK) bound of 5×10^{19} eV [2] may hint some unexpected results for the CR energy between $(\frac{1}{20} - 1) \times 10^{21}$ eV. Cosmic rays with $E > 5 \times 10^{19}$ eV have been observed [3], and hence the energy scale beyond $\gtrsim 100$ GeV (including the GZK bound) attracts a

¹Throughout this book, we use the word “Higgs boson” instead of “BEHGHK boson”, for simplicity.

h 125 GeV BEH boson	W^+ 80 GeV	u 2.5 MeV	c 1.3 GeV	t 173 GeV	χ ??? WIMP
	Z^0 91 GeV	d 5 MeV	s 95 MeV	b 4.2 GeV	
	W^- 80 GeV	ν_e < 0.1 eV	ν_μ < 0.1 eV	ν_τ < 0.1 eV	
	γ 0 eV Gauge bosons	e 0.5 MeV	μ 106 MeV	τ 1.8 GeV Quarks and leptons	
					$\langle a \rangle$??? Axion

Fig. 1.1. Elementary particles.

great deal of attention both in particle physics and astroparticle physics communities, in the PAMELA, Fermi, and AMS collaborations.

In a typical galaxy, stars are mostly on the galactic plane with a huge mass in the center. If these stars in the galactic bulge were the leading contributor to the gravitational pull of distant stars, the transverse velocity of a distant star at radius r from the galactic center falls as $1/\sqrt{r}$. But, the rotation curve shows “flatness” for large r [4]. This might hint at a dominant contributor to the gravitational pull not by stars, but by invisible mass, called DM in galaxies, as Zwicky speculated in the Coma Cluster. In recent years, galactic-scale DM has also been observed via the effect of gravitational lensing of electromagnetic waves coming from distant galaxies passing through galaxies in the line of sight.

From the particle physics point of view, the most profound evidence on DM comes from the history of the Universe. In the beyond the SM (BSM) physics, the SM singlet fields are introduced to understand some theoretical questions in cosmology and particle physics. Depending on the temperature below which these particles behave like DM, it is called hot if the particles are relativistic, cold if nonrelativistic,² or warm if they are in the interim region. In the standard Big Bang cosmology, one can estimate the energy densities of hot and cold DMs which were known to be a fraction of the critical density of the Universe since 1998. The critical energy density is the *current* average energy density for the Universe to be just flat,

$$\begin{aligned}
 \rho_c &\simeq 1.88 \times 10^{-29} h^2 \text{ g cm}^{-3} = 0.81 \times 10^{-46} h^2 \text{ GeV}^4 \\
 &\simeq 3.75 \times 10^{-47} \text{ GeV}^4 \quad (\text{for } h = 0.68).
 \end{aligned}
 \tag{1.1}$$

²Or, by the time of structure formation, it is cold because the effect of its velocity dispersion is negligible then.

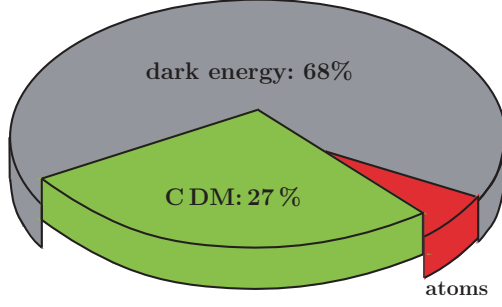


Fig. 1.2. Cosmic energy pie.

The energy density near our Sun is estimated to be 10^{5-6} times ρ_c . The fraction of cosmic energy of i , Ω_i , is compared to ρ_c : $\Omega_i = \rho_i/\rho_c$. The energy pie in the present Universe reported in 2013 splits into atoms constituting about 5%, cold dark matter (CDM) constituting about 27%, and the rest 68% being (presently unknown) dark energy (DE) [8], as shown in Fig. 1.2.

1.1.1. *Atoms*

Energy of atoms is mostly that of protons and neutrons in the nuclei, which are called baryons. When enough baryons are condensed in the Universe, they shine as stars. Observed lights from stars account for only $O(1\%)$ in the energy pie. Between stars and galaxies, there is gas of hydrogen. Adding these, baryons constitute about 5% in the energy pie. There can be small stars, e.g., of the Jupiter size, which do not shine. This kind of nonshining massive astrophysical compact halo objects (MACHOs) may behave like CDM. MACHOs are composed of baryons and electrons. By gravitational lensing, MACHOs can be searched for with the Hubble Telescope and with proper motion surveys. These searches have ruled out the possibility that MACHOs make up a significant fraction of DM in our galaxy [5]. The estimate of the baryon number density by the primordial nucleosynthesis process gives $0.021 \leq \Omega_B h^2 (= \eta_{10}/274) \leq 0.025$ with $5.7 \leq \eta_{10} \leq 6.7$ with 95% confidence limit [6]. Since $\Omega_c h^2 \simeq 0.12 h^2$, baryons can compose about 5% in the energy pie. Of course, this number includes MACHOs and interstellar gases. The recent observation [7] of gravitational waves by the LIGO group implies the merging of two massive black holes, $36M_\odot$ and $29M_\odot$, and there may be more black holes than speculated before. But, these nonluminous black holes must be included in the nucleosynthesis value of Ω_B and cannot be counted in the DM portion in the energy pie.

1.1.2. *Dark matter*

In the evolution of the Universe, radiation was decoupled from protons. Protons did not play a major role in the galaxy formation. Protons and electrons recombine to form atomic nuclei around the recombination time after the Big Bang. Before

the recombination time (t_{rec}), protons were in thermal equilibrium with photons and the proton inhomogeneity could not grow. This is because of the Silk damping [9], which is also called “photon diffusion damping”. The Silk damping reduced density inequalities (anisotropies) of protons greatly in the early Universe when protons were in thermal equilibrium with photons. Diffusion damping exponentially decreases anisotropies in the cosmic microwave background radiation (CMBR) on the Silk scale which is approximately $\lesssim 3 \text{ Mpc}$ much smaller than a degree. The mass contained within the Silk scale is the Silk mass. The Silk mass is estimated to be in the order of 10^{13} solar masses at the recombination time [10]. This mass is in the order of the mass scales of a present day galaxy or galaxy clusters. This scale, corresponding to the size of observed galaxies, implies that photon diffusion damping is responsible for *limiting the size of galaxies*. Since the proton inhomogeneity could not have grown before the recombination time, the inhomogeneity of the galaxy mass scales at the recombination time must have been produced by matter already decoupled from photons much before the recombination time. Cold DM is suggested for this role [11]. CDM was growing linearly since the cosmic time $t \approx 10^{10} \text{ s}$. Sometime after t_{rec} , the growing rate became nonlinear and gravitationally bound mass clumps were formed. The clumps of CDM produced in this way became the galaxies that we see today, by attracting protons after t_{rec} . These have been observed as temperature anisotropies by COBE [12], WMAP [13], and Planck satellites [8]. The WMAP and Planck satellite experiments have accurately given the temperature anisotropies at the order $\Delta T/T = \mathcal{O}(10^{-5})$.

The scale “Seed of CDM candidates” in Fig. 1.3 is the scale when both the CDM and baryon densities are determined. For a presentation purpose, we placed it after the nucleosynthesis era.

This astrophysical evidence in favor of the existence of CDM has grown over the years [14]. If CDM has provided the Silk scale at the time when CDM fluctuation enters into the horizon after inflation, the fluctuation scale is given by that horizon scale. This scale is typically the scale of galaxies. The density perturbation $\delta\rho$, a little bit larger than the average value, corresponding to $\delta\rho/\rho \simeq 3 \times \Delta T/T \simeq 3 \times 10^{-5}$, will become galaxies. The time scale corresponding to this is about 3×10^{-5} , i.e., the time at $z \simeq 3000$. Moreover $z \simeq 3000$ must be near the time when “matter = radiation”, since the density perturbation has grown only logarithmically before the time of “matter = radiation”. Since the time of $z = 10$, that pre-galaxy would remain at the same scale, attract baryons and would be shining later, but the horizon scale has kept increasing. The mass inside the Silk scale at the recombination time is the Silk mass.

The first hint for DM inferred by Zwicky in 1933 [1] came from the observation of velocity dispersion of the galaxies in the Coma Cluster. Still, the so-called the rotation curve in the halo forms the most convincing argument for the existence of

DM.³ If all the galaxy mass is inside the galactic bulge, which seems to be a good ansatz for shining stars, the rotation velocity of a star at r far from the bulge goes like

$$v(r) \propto \frac{1}{\sqrt{r}}. \quad (1.2)$$

This feature Eq. (1.2) is also confirmed by the revolution speeds of gas clouds of spiral galaxies [17].

Nevertheless, since all the evidence is based (directly or indirectly) solely on gravitational effects, we still do not know what the DM is actually composed of. In this book, we will discuss plausible candidates of CDM, which are consistent with particle theory.

1.1.3. *Dark energy*

Theoretical interpretation of dark energy (DE) can be related to the cosmological constant, originally introduced by Einstein [18]. But there has been a theoretical prejudice that the cosmological constant must be zero, which is considered to be one of the most important problems in theoretical physics [19]. After the introduction of fundamental scalars in particle physics, the vacuum energy of scalar fields has been appreciated to contribute to the cosmological constant [20]. Therefore, the problem related to the cosmological constant must be considered together with the vacuum energy of scalar fields.

Some properties of the Universe provide further evidences, as to its structure and history. The age of our Universe, 13.8 billion years, is very long: if the matter density were too high, one would expect it to have gravitationally collapsed on itself, while if DE density were too high, then one would expect that accelerated expansion would have removed all stars and galaxies to beyond our purview [19]. Measurements of the CMBR [8] imply that the Universe on large scales is homogeneous and isotropic to one part in 10^5 [12]: this is surprisingly smooth for apparently causally disconnected regions. Yet, on smaller scales the Universe appears quite lumpy: inhomogeneous and anisotropic, the seed of which was provided by CDM. To understand the large-scale smoothness, it is hypothesized that the Universe has gone through an early inflationary epoch of rapid expansion so that the seemingly disconnected regions were in fact causally connected before through the inflation history. Only a tiny matter density existed at the end of inflation [21–24]. To understand the small-scale inhomogeneities, it is required that quantum fluctuations before inflation provided the seeds to allow the Universe to have gone through a gravitational

³Of course, one could obtain the flat rotation curves by changing gravity on different scales, called modified Newtonian dynamics (MOND) [15], which is not emphasized in this book. It is discussed in Vol. 3 of this Encyclopedia [16].

condensation phase, so galaxies, stars, planets and ultimately life forms could have arisen [25].

Inflation predicts that the total mass–energy density of the Universe is very close to the critical closure density $\rho_c = 3H_0^2/8\pi G_N \simeq 1.88 \times 10^{-29} h^2 \text{ g cm}^{-3}$, where G_N stands for the gravitational constant and H_0 denotes the current value of the Hubble parameter which is parameterized as $H_0 \equiv 100 h \text{ km/sec/Mpc}$ and $h \simeq 0.674$ [8]. The recent WMAP [13] and Planck [8] satellite data confirm that the energy density of the Universe is nearly ρ_c (spatially flat) and that the present DE is about 68% of the critical energy density of the Universe. The simplest form of DE is the so-called cosmological constant. The WMAP/Planck data fit, to the Λ CDM cosmological model (supported by data from galactic rotation curves, weak lensing measurements, baryon acoustic oscillations, etc.), implies that the matter density in the Universe lies at the $\sim 32\%$ of closure density level of which about 5% lies in baryonic matter while $\sim 27\%$ constitutes CDM as shown in Fig. 1.2.

1.2. Cosmic history

The WMAP collaboration has provided an intuitive cartoon shown on the left-hand side of Fig. 1.3. An observer at present sees light coming from the recombination time when photons were decoupled from electrons and freely traveled up to our telescopes. The cartoon on the right-hand side looks deep into the past to the last scattering surface at the time of recombination. The size of galaxies, represented as the size of temperature perturbations [8, 13], is the one coming from the last scattering surface, i.e., at the time after recombination. The size of gravitationally condensed galaxies did not grow after this time, except mergers, but the horizon scales continued to grow, from the time of $z \approx 10^3$ (recombination time) to $z = 0$ (present), and the scale factor increased by $O(10^3)$, leading to an opening angle of order 0.2 degrees. In Fig. 1.3, a typical opening angle is shown with a great exaggeration. This cartoon is drawn under the following assumptions and theories.

Without a correct quantum gravity theory, we assume the beginning of the Universe is some time after the Planck time, 10^{-43} s . In the very early Universe, the Universe has gone into the high-scale inflationary phase. The high-scale inflation might not be ruled out yet, and attracted a great deal of attention recently [26, 27]. The high-scale inflationary epoch ended after rolling on a flat curve on top of $V \simeq (10^{15-16} \text{ GeV})^4$, ending at the cosmic time around $t^{-1} \simeq H_I \simeq 10^{14} \text{ GeV}$. The next notable cosmic event occurred at the time of nucleosynthesis, having begun at the time of neutrino decoupling at temperature $T_{\text{dec}}^\nu \simeq 1 \text{ MeV}$. However, to manufacture helium-4, ${}^4\text{He}$, the Universe must have gone through the deuterium bottleneck period, after which the temperature fell down to 0.1 MeV. Then, after the temperature dropped down to $\approx (10\text{--}100) \text{ eV}$, the (present) galactic-scale entered into the horizon which has remained almost the same until now. Within this scale, CDM particles fell in and massive lumps of this order of scale became gravitationally

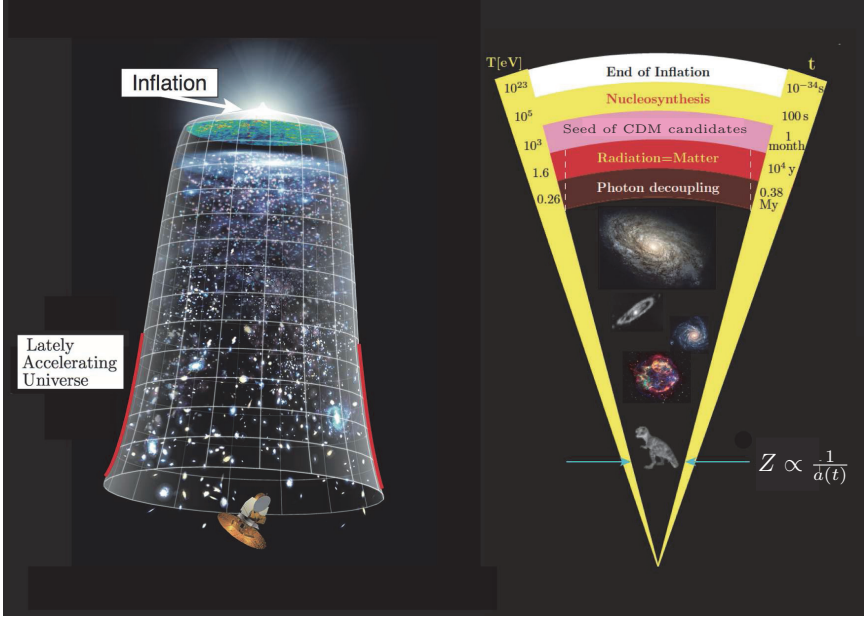


Fig. 1.3. A cosmic history based on the Λ CDM model.

bound structures and did not expand via the Hubble law. These gravitationally bound structures can be viewed as point masses distributed homogeneously in the expanding Universe. Thus, CDM is the seed for making some habitable places of life — galaxies. This scale for seed of galaxies is marked as “Seed of CDM candidates”. It was still in the radiation-dominated epoch. Then, after some time matter density took over the radiation density, which is marked as “radiation = matter”. This is called the matter–radiation equality point. It occurred 10,000 years after the Bang. Next, after 380,000 years, photons were decoupled and suddenly the Universe became dark, entering into the dark age of the Universe. A good time unit since then until the extinction of dinosaurs at 65 million years ago was 0.1 billion (i.e., 100 million) years. Let us call this unit 1 Ey,⁴ i.e., the Universe was born 138 Ey ago.

The dark age continued for some time until the born of the first stars. Since the age of Sun is 46 Ey and globular clusters are older than 100 Ey, the first stars were probably born at the Universe age of less than 20 Ey. After the first stars were born, the sky was filled with lights from stars in Milky Way, and lights from groups of stars in distant galaxies. These galaxies are marked in Fig. 1.3, with the first galaxy size schematically shown below the recombination line. After the Universe age of 92 Ey, Sun and Earth were born and geophysics deals with the evolution of Earth (since 45 Ey), including the birth of life forms.

⁴E is 10^8 = hundred million.

In this history, two important events for our existence are the epochs of “CDM density fixed” and “matter–radiation equality” by which our galactic home was created. The first condition is determined by interactions of particles, including the mechanisms for baryogenesis and creation of CDM, and the second is obtained from Einstein’s gravity, on the anisotropy in the RHS of the Einstein equation, $\delta\rho/\rho$.

1.3. A survey of candidates for DM particles

The basic reason for Silk damping was the inhibition of photons to propagate a long distance in the presence of electromagnetically charged particles. So, the conditions that the DM particle candidates satisfy are:

- (1) nonbaryonic, i.e., carrying neither electric nor (preferably) color charges;
- (2) stable (or at least extremely long lived, with the lifetime exceeding the age of the Universe by many orders of magnitude);
- (3) nonrelativistic (and thus massive) since relativistic particles (such as neutrinos) would exceed the escape velocity of clumping baryons and thus could not produce the gravitational wells needed for structure formation.

While some DM candidates are mentioned just to fit the DM density, others emerge quite naturally from solutions to long-standing problems in particle physics. In this latter category, notable candidates include the “invisible” axion [28], which emerges from the Peccei–Quinn solution [29] to the strong CP problem; and the neutralino [30] which emerges from a supersymmetric (SUSY) solution to the gauge hierarchy problem. In cases such as these and others, the relic abundance of DM along with DM detection rates are calculable in terms of fundamental parameters, and thus subject to experimental searches and tests.

Generally, DM relics are considered to be produced in the early Universe in (at least) two distinct ways. One possibility involves DM particles generated in processes taking place in thermal equilibrium, which we will generically refer to as *thermal production* (TP), and the relics produced this way will be called *thermal relics*. On the other hand, *nonthermal production* will refer to processes taking place outside of the thermal equilibrium, and the resulting relics will be called *nonthermal relics*. The first class of processes will include the freeze-out of relics from thermal equilibrium, or their production in scatterings and decays of other particles in the plasma. The second will include, for example, relic production from bosonic coherent motion (BCM).

The most often considered theoretical candidate for CDM is the weakly interacting massive particle (WIMP). It is worth stressing, however, that the WIMP is not a specific elementary particle, but rather a broad class of possible particles. Lee and Weinberg [31] introduced WIMPs in 1977 in the form of stable, massive left-handed neutrinos which could play the role of CDM. Such weakly interacting particles were excluded as CDM long ago due to lack of signal in direct DM detection experiments. Since then a whole host of various weakly interacting particles have

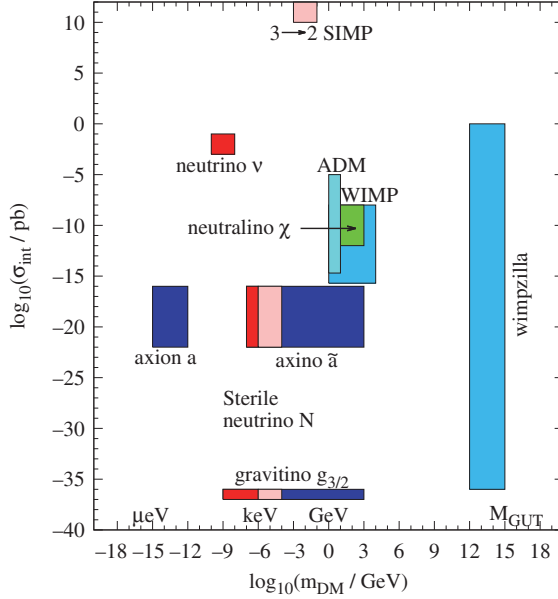


Fig. 1.4. Candidates of DM particles.

been discussed in the literature, many of these possibilities have now been excluded by experiment, although many also have so far survived experimental tests.

An overview of several well-motivated DM candidates are listed in Fig. 1.4 (taken from Ref. [32]) in the detection cross-section vs. mass plane. On the vertical axis, a typical order of magnitude detection cross-section associated with each type of candidate. For example, an SM neutrino with mass of order 0.1 eV and weak interaction strength of order $10^{-36} \text{ cm}^2 = 1 \text{ pb} \simeq 1 \text{ GeV}^{-2}/3.92$ is shown, although such a candidate would constitute hot DM and thus does not meet the above third condition. The candidate particles are the following:

- **Axion:** The box on axion is for the very light QCD axion [28]. The “invisible” axion solves the strong CP problem, a kind of hierarchy problem.
- **WIMP:** The box marked “WIMP” represents “generic” weakly interacting massive particle candidates from *thermal relics*. Their mass can lie in the range between a few GeV [31] (below which it would overclose the Universe) and some $\sim 100 \text{ TeV}$. The most highly scrutinized thermal relic is the lightest neutralino particle of SUSY theories [30], hereafter referred to as simply the neutralino. The neutralino is particularly well-motivated since, in addition to solving the DM problem, SUSY extensions of the SM contain a number of other attractive features both on the particle physics side and in the early Universe cosmology. In addition to the neutralino, there are a host of WIMPs suggested in the literature. These have the weak-scale scattering cross-sections with their masses from above a few GeV to the $\sim 1 \text{ TeV}$ scale, based on some suggested theoretical expectation. Mirror

DM, minimal DM, sterile neutrino or right-handed neutrino [31] all belong to this category. These will be discussed in more detail in Chapter 7.

- **E-WIMP:** The extremely weakly interacting massive particle is known as the E-WIMP. Sometimes the term feebly interacting massive particle is used for this category. The best known particle in this category is *axino* which is the super-partner of axion [32]. Axino can be hot [33], warm [34], or cold [35]. Axinos can be either thermal or nonthermal relics, or both, since they can be produced in both thermal production and nonthermal processes.
- **Gravitino:** With SUSY, supergravity theory predicts the *gravitino* $\tilde{G}$, the fermionic partner of the graviton. It is another well-motivated example of an E-WIMP. Gravitino can be hot [11], warm [34], or cold [36], as distinguished by colors in Fig. 1.4.
- **Other BSM particles:** Any long-lived particle beyond the SM spectrum, in addition to those discussed above, has a potential to become DM. Theoretically, some (almost-) exact discrete symmetries such as $\mathbf{Z}_2$ are employed for this purpose.
- **Particles with extra forces:** Other than discrete symmetries, extra gauge interactions can also be considered belonging to the BSM. There have been many proposals for new gauge interactions, mainly working in the dark sector. The most well-known one is the dark force presented in Ref. [37]. Here, some stable elementary or composite particle can be a candidate for a DM particle.
- **ADM:** Conservation of asymmetric DM particles is similar to the conservation of baryon number B . So, one introduces a global symmetry $U(1)_{\text{ADM}}$ and follows the method of creating B in the standard Big Bang cosmology [38].
- **Wimpzilla:** In inflationary cosmology, reheating is the follow-up process. During the reheating process, some supermassive particles can be considered to be DM candidates which are called Wimpzillas [39].
- **Q-balls:** Some Q-balls, which are non-topological solitons, can be candidates of DM if they are stable [40]. Global symmetries are the underlying symmetry because one needs large number of charges in the Q-balls.
- **Primordial black holes:** Primordial black holes formed before nucleosynthesis and surviving now can work as DM portion in the cosmic energy pie. Based on the estimation on the density of these black holes, there is some constraint on this possibility [41].

But there are much more theoretical ideas for DM as shown with a cartoon in Fig. 1.5 [42]. Among these, we have concentrated to those directly related to symmetry principles.

1.3.1. *WIMP miracle?*

As one can see from Fig. 1.4, particle relics with a correct relic density span a mass range of some 33 orders of magnitude, while interaction cross-sections range

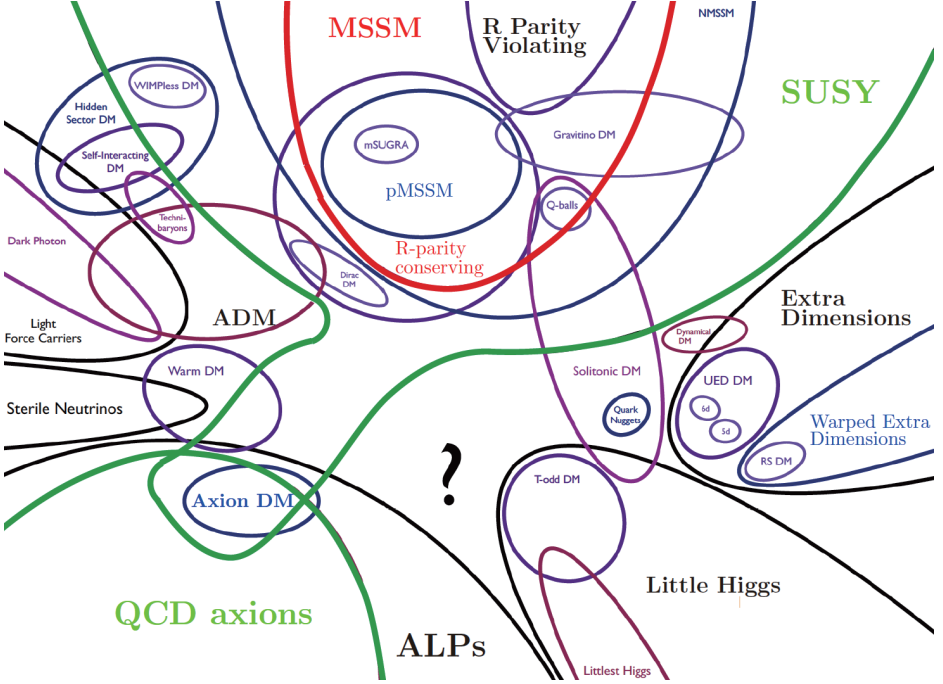


Fig. 1.5. Theoretical ideas for DM.

across over 40 orders of magnitude. This is possible because their populations can be generated by very different production mechanisms in the early Universe. Of the possible DM candidates, WIMPs as thermal relics remain, however, the most scrutinized possibility for DM due to a conspicuous connection between the CDM relic density and the electroweak interaction strength. The argument, often referred to as the WIMP “miracle”, goes as follows. In the early Universe WIMPs (denoted by X) are assumed to be in thermal equilibrium at temperature $T \gtrsim m_X$. The WIMP number density n_X as a function of time t is governed by the Boltzmann equation

$$\frac{dn_X}{dt} = -3Hn_X - \langle \sigma_{\text{ann}} v \rangle (n_X^2 - n_{\text{eq}}^2). \quad (1.3)$$

Here n_{eq} is the equilibrium density, H the Hubble constant for a radiation-dominated Universe is given by $H^2 = \rho_{\text{rad}}/3M_P^2$, and $\langle \sigma_{\text{ann}} v \rangle$ denotes the thermally averaged WIMP annihilation cross-section times WIMP relative velocity. At early times, the number density tracks the equilibrium density. However, at some point — known as the freeze-out point at the temperature T_{fr} — the expansion rate outstrips the annihilation rate and the Hubble term becomes dominant. At that point, the WIMPs freeze-out and their number density in a comoving (expanding) volume becomes effectively constant.

An approximate solution of the Boltzmann equation provides the present day WIMP relic density as

$$\Omega h^2 \simeq \frac{s_0}{\rho_c/h^2} \left(\frac{45}{\pi^2 g_*} \right)^{1/2} \frac{1}{x_f M_P} \frac{1}{\langle \sigma_{\text{ann}} v \rangle}, \quad (1.4)$$

where s_0 denotes the present day entropy density of the Universe, g_* the number of relativistic degrees of freedom at freeze-out and $x_f \equiv T_{\text{fr}}/m_X \sim 1/25$ the freeze-out temperature scaled to m_X (for a derivation, see Section 2.2). Plugging in the known values [43] for s_0 , ρ_c and M_P and setting $\Omega_\chi h^2$ to its measured value $\simeq 0.12$, one finds

$$\frac{\Omega h^2}{0.12} \simeq \frac{1}{\frac{\langle \sigma_{\text{ann}} \rangle}{10^{-36} \text{cm}^2} \frac{v/c}{0.1}}. \quad (1.5)$$

Thus, an annihilation cross-section of weak strength of order $\sim 10^{-36} \text{cm}^2$ ($= 1 \text{ pb}$) and typical WIMP velocities at freeze-out give the correct present day relic density of DM. This remarkable number related to the weak interaction cross-section is called a “miracle”.

1.4. The scope of this volume

Dark matter is the subject relating particle physics, astrophysics and cosmology. In Chapter 2, an overall view on DM is presented. In Chapter 3, the astrophysical hints on DM are presented together with a short discussion on the density fluctuations as the source of large-scale structures in the Universe, where most DM particles are located. In Chapter 4, the symmetry principles, which are the bases of DM, are presented. In particular, the SM of particle physics and its extension to the BSMs are discussed. In Chapter 5, extended objects in cosmology are discussed. In Chapter 6, the bosonic collective motions, which include the QCD axion, are presented. In Chapter 7, massive DM particle candidates, which includes the WIMP, are discussed. In Chapter 8, “baryogenesis”, which can be applicable to the asymmetric DM, is discussed. Finally, in Chapter 9, efforts in the experimental search of DM particles are presented. Galaxy formation, numerical simulation, and DE are discussed in more detail in other volumes of this Encyclopedia [16, 44].

1.5. Notation

The symbols used in this book are shown on page xii.

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Chapter 2

Dark Matter Production in the Universe

*Things should be made as simple as possible,
but not any simpler — A. Einstein*

2.1. Basics

As introduced in the previous chapter, there are two well-known candidates for CDM, the bosonic coherent motion (BCM) and the weakly interacting massive particle (WIMP). The Universe evolves in the presence of these CDM components. The governing equation for the large-scale structure of the Universe is the Einstein equation

$$\mathcal{R}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} \mathcal{R} = 8\pi G_N T_{\mu\nu} - \Lambda g_{\mu\nu}, \quad (2.1)$$

where $\mathcal{R}_{\mu\nu}$ ($\mathcal{R}$) is the Riemann tensor (Ricci scalar), $T_{\mu\nu}$ is the energy–momentum tensor, Λ is Einstein’s cosmological constant [1], and $M_{\text{P}} = \sqrt{1/8\pi G_N} \simeq 2.44 \times 10^{18} \text{ GeV}$ is the reduced Planck mass. For the case of WIMP, its contribution is only through its amount in $T_{\mu\nu}$, via mass times the number density, which depends on the cosmic time t . On the other hand, in the evolving Universe, the BCM case is further constrained by its equation of motion.

2.1.1. *Friedmann–Lemaître–Robertson–Walker Universe*

For a homogeneous and isotropic Universe, the metric is given by the Friedmann–Lemaître–Robertson–Walker (FLRW) form,

$$ds^2 = dt^2 - a^2(t) \left\{ \frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2 \right\}, \quad (2.2)$$

where $a(t)$ is the scale factor and k is the 3-space curvature which is equal to -1 , 0 or 1 for an open, flat or closed Universe, respectively. In the FLRW Universe, only the scale factor $a(t)$ in the metric is a function of time,¹ and in this spatially homogeneous Universe, $T^{\mu\nu}$ is expressed in terms of two functions, the energy density $\rho(t)$ and the pressure $p(t)$,

$$T^{\mu\nu} = (\rho + p)U^\mu U^\nu + pg^{\mu\nu}, \quad (2.3)$$

where U^μ is the fluid four-vector velocity and the momentum conservation law $T^{i\mu}_{;\mu}$ is automatically satisfied with the FLRW metric. It becomes

$$T^{\mu\nu} = \begin{pmatrix} \rho(t) & 0 \\ 0 & \tilde{g}^{ij}a^{-2}(t)p(t) \end{pmatrix}, \quad (2.4)$$

in the rest frame of fluid. On the other hand, the continuity equation of $T^{0\mu}$ becomes

$$\begin{aligned} T^{0\mu}_{;\mu} &= \frac{\partial T^{0\mu}}{\partial x^\mu} + \Gamma^0_{\mu\nu}T^{\nu\mu} + \Gamma^\mu_{\mu\nu}T^{0\nu} \\ &= \frac{\partial T^{00}}{\partial t} + \Gamma^0_{ij}T^{ij} + \Gamma^i_{i0}T^{00} = \frac{d\rho}{dt} + 3(\rho + p)\frac{\dot{a}}{a} = 0. \end{aligned} \quad (2.5)$$

Here, we introduce the Hubble parameter $H \equiv \dot{a}/a$. The scale factor $a(t)$ is related to the redshift z by

$$a(t) = \frac{1}{1+z(t)}, \text{ with } a(t_0) = 1. \quad (2.6)$$

The conservation equation for the energy density ρ becomes

$$\dot{\rho} + 3H(\rho + p) = 0. \quad (2.7)$$

The evolution of $a(t)$ is given by

$$H^2 = \frac{\rho}{3M_{\text{P}}^2} + \frac{\Lambda}{3} - \frac{k}{a^2}. \quad (2.8)$$

Differentiating (2.8) with respect to t ,

$$2H\dot{H} = \frac{\dot{\rho}}{3M_{\text{P}}^2} + 2k\frac{\dot{a}}{a^3} = \frac{H}{M_{\text{P}}^2} \left(-\rho - p + \frac{2kM_{\text{P}}^2}{a^2} \right) \quad (2.9)$$

or

$$\frac{\ddot{a}}{a} = -\frac{1}{6M_{\text{P}}^2}(\rho + 3p) + \frac{\Lambda}{3}. \quad (2.10)$$

Since ρ is positive, an accelerating Universe needs $-\frac{p}{2M_{\text{P}}^2} + \frac{\Lambda}{3} > 0$, i.e., negative pressure in cases of negligible ρ and Λ . The recent acceleration observed in 1998 [2]

¹In this book, a is used both for the scale factor and the axion field.

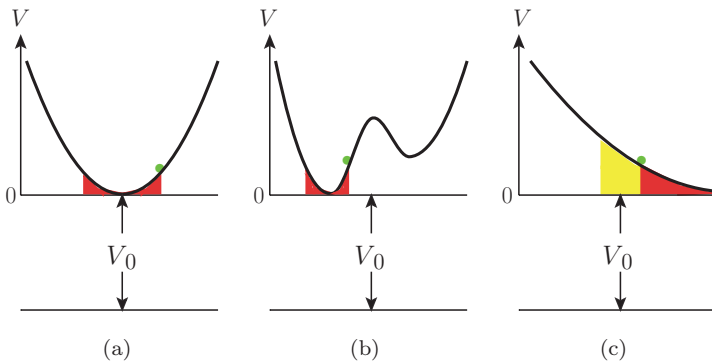


Fig. 2.1. The possibilities of V bounded from below: (a) a unique minimum, (b) several local minima, and (c) no local minimum. We can consider these shapes for high-scale inflation (except case (c)) and also for the recent acceleration. In the latter case, colored regions are commented in the text.

requires negative pressure which is interpreted as DE [3]. In addition to this DE, the matter component contributes in Eq. (2.3) as $\rho(t) > 0$ and $p(t) = 0$ component. A small cosmological constant about two and a half times ρ_{CDM} is sufficient for this.

In Eq. (2.10), the positive pressure is interpreted as the attractive force for the metric, influencing as $\ddot{a} < 0$; and then negative pressure corresponds to the repulsive force with $\ddot{a} > 0$. In Eq. (2.8) ρ includes energies due to atoms and CDM. For a WIMP with large mass, its velocity is negligible at low cosmic temperature. So, $p(t)$ of the WIMP at late cosmic time is considered to be almost zero. In this case, Eq. (2.7) implies $(d/dt)(\rho a^{3(1+\omega)}) = 0 \rightarrow \rho a^3 = \text{constant}$ for $\omega = 0$.

2.1.2. Energy forms

For cosmological constant Λ_{cc} in $\int d^4x (-\frac{M_{\text{p}}^2}{2} \mathcal{R} + \Lambda_{\text{cc}})$, the energy-momentum tensor has the form $-g^{\mu\nu} \Lambda_{\text{cc}}$, i.e., $p = -\rho$ is negative and there results an accelerating Universe. In fact, Eq. (2.7) with $p = -\rho$ gives a constant ρ and Eq. (2.8), neglecting the k term, gives an exponentially expanding Universe

$$a(t) = a(t_0) e^{H(t-t_0)}. \quad (2.11)$$

For the accelerating Universe, we must include Λ in Eq. (2.10) and the vacuum energy contributed by scalar fields. For simplicity, let us consider only one scalar field. In Fig. 2.1, we draw possible situations of bounded potentials of a scalar ϕ . Here, Fig. 2.1(c) corresponds to a potential of a scalar field sliding to infinity. In each case, we marked two horizontal lines for the values of V : one at 0 and the other at $-V_0$. Here $-V_0$ is a reference point for the origin of V . Without considering gravity, we can choose any value for $-V_0$, even a positive value in the figure. Here, we set $-V_0 = 0$.

In Fig. 2.1, the field energy above the line 0 is denoted as $\mathbf{V}_\phi$. When the field ϕ oscillates as BCM [4], it behaves like CDM. So, our CDM energy is the sum of energies of this BCM and WIMPs. CDM is important in the current phase in the evolution of the Universe. We can distinguish several cosmic epochs as follows:

- (I) very early Universe, epoch of inflation;
 - (II) early Universe, epoch of radiation/matter-dominated period;
 - (III) late Universe, epoch after $\text{DE} \approx \text{CDM}$: *current phase*;
 - (IV) future Universe, epoch after $\text{DE} \gtrsim 100$ times CDM.
- (2.12)

In this Encyclopedia, phase (I) is discussed in each volume for its purpose, and phase (II) is discussed in Volume 1. Phase (III) is discussed in Volume 3 and here. Phase (IV) is the fate of our Universe.

2.1.3. *Future*

In Eq. (2.12), the equation of state is used to obtain the time dependence of the Hubble parameter by the relation

$$\rho_i \propto a(t)^{-n_i}, \quad \text{or} \quad \rho_i \propto T^{n_i}. \quad (2.13)$$

Then, we have

$$\frac{\Omega_i}{\Omega_j} \propto a(t)^{-(n_i - n_j)}, \quad (2.14)$$

where the energy fraction of species i is the ratio relative to the critical energy density ρ_{crit} ,

$$\Omega_i = \frac{\rho_i}{\rho_{\text{crit}}}. \quad (2.15)$$

The species i has parameters n_i and w_i as presented in Table 2.1, where w_i is defined as

$$w_i = \frac{p_i}{\rho_j}, \quad (2.16)$$

which distinguishes the cosmic epochs. From Table 2.1, we have the relation

$$n_i = 3(1 + w_i). \quad (2.17)$$

Table 2.1. n_i and w_i of species i .

Species	n_i	w_i
Matter	3	0
Radiation	4	$\frac{1}{3}$
“Curvature”	2	$\frac{-1}{3}$
Vacuum	0	-1

From Eqs. (2.8) and (2.10), we obtain the following relations in the flat space,

$$-\frac{\ddot{a}}{a} = \frac{1}{6M_{\text{P}}^2} \sum_i \rho_i n_i - \frac{1}{3} \Lambda, \quad (2.18)$$

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{1}{3M_{\text{P}}^2} \sum_i \rho_i + \frac{1}{3} \Lambda \rightarrow \frac{1}{3M_{\text{P}}^2} \rho_{\text{crit}}. \quad (2.19)$$

Thus, we obtain

$$\frac{-\ddot{a}/a}{H^2} = \frac{1}{2} \left(\sum_i \frac{\rho_i n_i}{\rho_{\text{crit}}} - 2 \frac{\Lambda M_{\text{P}}^2}{\rho_{\text{crit}}} \right). \quad (2.20)$$

In addition to the Hubble parameter, the deceleration parameter q is an important parameter describing the evolution of the Universe,

$$q = -\frac{\ddot{a}a}{\dot{a}^2}, \quad (2.21)$$

which is given from the n_i entries of Table 2.1, which is in fact given in Eq. (2.20),

$$q = \sum_i \frac{n_i - 2}{2} \Omega_i = \frac{1}{2} \Omega_{\text{M}} - \Omega_{\Lambda}. \quad (2.22)$$

If $V_0 \neq 0$ in Fig. 2.1, the future evolution of our Universe is shown in Fig. 2.2 [5]. If $\Lambda_{\text{cc}} > 0$ as discussed in many vacuum energy models, the point $(\Omega_{\text{M}}, \Omega_{\text{DE}}) = (0, 1)$ is the de Sitter space fixed point of the convergence shown as the red bullet. The current values of Ω_{M} and Ω_{DE} are marked as a star. If Ω_{DE} is indeed the cosmological constant Λ_{cc} , our future evolution is shown as the red arrow. In this case, our Milky Way will be a lonely one in the far future, deprived of any light from other galaxies. But the current value of DE can be due to vacuum energy of a scalar field with $\Lambda_{\text{cc}} = 0$ [6]. Then, in the far future, the evolution follows the dashed line shown in Fig. 2.2.

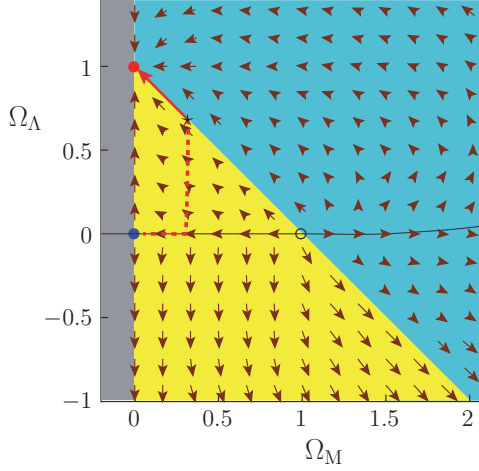


Fig. 2.2. Dynamics for Ω_Λ and Ω_M . Arrows show the direction of the evolution of Ω_Λ and Ω_M . Above the recollapse line, the Universe will expand forever, corresponding to the fixed point, the red bullet. It needs $\Omega_\Lambda > 0$. Our Universe, marked as a star, will end up at this de Sitter fixed point in the future. But, if $\Omega_\Lambda \simeq 0.7$ is temporary as in the quintessential axion model [6], the future will follow the red dashed line.

2.1.4. Density perturbation

The density perturbation $\delta\rho/\rho$ enters into the Einstein equation, Eq. (2.1), on the right-hand side (RHS). It is derived from a perturbation on the quantum field $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$. The metric acts as a gravitational potential and $\delta\rho/\rho$ is developed in this potential.

Let $\ell_{\Delta g}$ be the quantum fluctuation scale of $g_{\mu\nu}$. If the scale $\ell_{\Delta g}$ enters into the inflationary period [7, 8], it stays fixed like a fossil during inflation. Even after the inflation, the scale is treated as fixed if the scale is larger than the horizon scale. If $\ell_{\Delta g}$ re-enters into the horizon, the full tensors $T_{\mu\nu}$ inside $\ell_{\Delta g}$ are correlated. These event points are shown in Fig. 2.3. After the re-entry into the horizon, the CDM particles move toward the galactic center following the gravitational potential Δg . Thus, the galactic scale of order $\ell_{\Delta g}$ is generated. It occurred at the time “CDM density fixed” in Fig. 2.3.

Quantum fluctuations of massive particles are limited to their Compton wavelengths, and hence they are not cosmologically important. But, any massless quantum field might have had quantum fluctuations of cosmological interest. Note that the photon cannot work for this purpose because of the gauge symmetry.² But, some Goldstone bosons might have this cosmological effect of entering into the inflationary phase and the re-entry into the horizon.

²The basic difference between gauge bosons and Goldstone bosons in gravity is emphasized in later chapters.

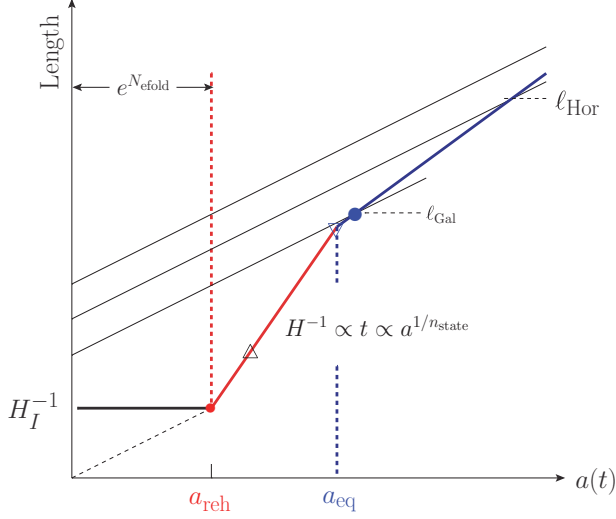


Fig. 2.3. The scales of H^{-1} . The horizon after inflation is marked as thick red and blue lines. The open uptriangle is the time when CDM density is fixed, i.e., “Seed of CDM candidates” in Fig. 1.3. The open downtriangle is the point of “matter = radiation” at a_{eq} . The blue bullet is the point when the CDM density fluctuation entered into the nonlinear regime. The region around the blue bullet is shown in Fig. 3.9. Here a_{reh} is the scale when the radiation-dominated Universe commenced after inflation. The cosmic time vs. the scale factor slope n_{state} is 2 and 1.5 in the RD and MD Universes, respectively. The e-fold number via inflation is N_{efold} .

Among the CDM candidates, some scalar fields such as BCM can be considered for this possibility. Thus, the quantum fluctuations of Goldstone bosons can also be considered [4]. The best worked out example is the axion a [9]. So, quantum fluctuations of the quantum field a also follow the same scenario of entering into the inflationary period and re-entering into the horizon. Along this line, a severe isocurvature constraint was used to limit the axion mass [10, 11], which narrowed down the axion window further. In this region for the QCD axion, the re-entry temperature is about 1 eV, after the nucleosynthesis epoch in Fig. 1.3. The time for “CDM density fixed” of Fig. 2.3 has its origin at the “Seed of CDM candidates” of Fig. 1.3, which can be much earlier in the case of WIMPs. Therefore, by the time of “CDM density fixed”, the axion oscillation $\langle a(t) \rangle$ works as CDM and the axion fluctuation scale at its re-entry time is the relevant scale at the time. But, the seed of oscillating QCD axion is determined during the time of QCD phase transition marked as the uptriangle in Fig. 2.3. In this way, the QCD axion practically works as CDM now, like WIMP. Axions will be discussed more in Chapter 6.

The scale at the time of “CDM density fixed” in Fig. 2.3 determines the scale of galaxies. The density perturbation $\delta\rho$ a little bit larger than the average value, corresponding to $\delta\rho/\rho \simeq 3 \times \Delta T/T \simeq 3 \times 10^{-5}$, leads to galaxies. The time scale corresponding to this is about 3×10^{-5} the time at $z \simeq 10$, i.e., at $z = 3000$, which is a bit later than the time “matter = radiation” (at a_{eq} of Fig. 2.3), since the density

perturbation grew only logarithmically before the time of “matter = radiation”. Since the time of $z = 10$, that scale of pre-galaxy will remain at the same size, attract baryons and will be shining later, but the horizon scale has kept increasing. The mass inside the Silk scale, marked as the horizontal dashed line in Fig. 2.3 at ℓ_{Gal} , is the Silk mass.

2.2. Thermal production

2.2.1. Number density history

One can solve the Friedmann equation for each case of cosmic epochs of Eq. (2.12),

$$\text{Radiation-dominated (RD) phase:} \quad \rho \propto a^{-4}, \quad (2.23)$$

$$\text{Matter-dominated (MD) phase:} \quad \rho \propto a^{-3}, \quad (2.24)$$

$$\text{Cosmological constant dominated (CCD):} \quad \rho \propto \text{constant}. \quad (2.25)$$

The early Universe (phase (II) of (2.12)) right after inflation was dominated by relativistic particles (RD) and later on dominated by matter particles (MD). At the current phase, i.e., in the late Universe of (2.12), the Universe is accelerating and is dominated by DE (CCD) but there still exists a significant portion of CDM. In the far future Universe, CDM will be negligible compared to DE.

The initial inflationary period provides an explanation for the cosmological problems related to the initial conditions of the standard Big Bang cosmology (for a review, see, e.g., [7]). During inflation, the Universe became very flat and homogeneous with only small amounts of fluctuations. After inflation, the oscillating inflaton field Φ briefly makes the Universe matter-dominated until its decay produces relativistic particles: the Universe is then *reheated* and then begins the standard Big Bang Universe. This process is called *reheating*. If there exist particles which live long enough, with lifetime larger than 10^3 s, they affect the process of nucleosynthesis. Thus, the abundance of these massive particles after reheating is constrained. One such example is the heavy gravitino in supergravity models. Therefore, in supergravity theories, either the gravitino mass is constrained to be heavier than 10 TeV for the BBN to restart from scratch after the decay of gravitino [12],³ or the Universe is constrained to have the reheating temperature lower than 10^9 GeV [14].⁴ Somewhat below the reheating temperature T_{reh} , the Universe is described pretty well by the RD Universe.

³This bound comes from a BBN constraint that $T_{\text{reh}} > 0.7$ MeV. If hadrons are produced with $O(1)$ branching ratio by the gravitino decay, T_{reh} must be above (4–5) MeV for the hadrons to be thermalized with n and p [13].

⁴Hadrons by the gravitino decay have been considered to obtain a lower upper bound $T_{\text{reh}} < 10^7$ GeV in some models [15].

For simplicity, it is usually assumed that the particles produced from inflaton decay are thermalized instantly and the reheating temperature T_{reh} is defined as the temperature when the energy density of radiation dominates the matter density of the oscillating inflaton field [8, 16], i.e., T_{reh} is the maximum temperature attained *during the RD phase*. That happens around a time comparable to the lifetime of the inflaton field, $t \sim H^{-1} \simeq \tau = \Gamma_{\Phi}^{-1}$, when the inflaton energy density exponentially decreases. From the Friedmann equation, the reheating temperature can be expressed as

$$T_{\text{reh}} \simeq \left(\frac{90}{4\pi^2 g_*} \right)^{1/4} \sqrt{\Gamma_{\Phi} M_{\text{P}}}, \quad (2.26)$$

where g_* counts the effective number of relativistic species present in equilibrium. For photon, real scalar, neutrino, and electron, the effective numbers are

$$g^* = \begin{cases} 2 & \text{for } \gamma, \\ 1 & \text{for } \phi, \\ \frac{7}{8} & \text{for both } \nu \text{ and } \bar{\nu}, \\ \frac{7}{4} & \text{for both } e^- \text{ and } e^+. \end{cases} \quad (2.27)$$

However, the maximum temperature T_{max} (the highest temperature reached after inflation but which may be attained before the onset of RD) can be much higher than the reheating temperature [8, 17]. If the thermalization is delayed and occurs after RD, then the reheating temperature can be much lower than that defined by Eq. (2.26) [18, 19]. To maintain the successful predictions for the abundances of light nuclei production during the standard Big Bang nucleosynthesis (BBN), it is required that $T_{\text{reh}} \gtrsim 4 \text{ MeV}$ [20].

The early Universe after inflation was filled with relativistic particles in a plasma that was very hot and dense. The relativistic particles, collectively referred to as radiation, became thermalized due to their self-interactions thus reaching local thermodynamic equilibrium. From the equilibrium distributions, the energy density, number density and entropy density of radiation are, respectively, given by

$$\rho_R = \frac{\pi^2}{30} g_* T^4, \quad (2.28)$$

$$n_R = \frac{\zeta(3)}{\pi^2} g_* T^3, \quad (2.29)$$

and

$$s = \frac{2\pi^2}{45} g_* T^3, \quad (2.30)$$

where $\zeta(3) = 1.20206\dots$ is the Riemann zeta function of order 3, and g_{*S} denotes the effective degrees of freedom of entropy at the time of decoupling.

For the nonrelativistic particles in thermal equilibrium (e.g., WIMP, X), one finds

$$\rho_X = m_X n_X, \quad \text{with } n_X = g \frac{(m_X T)^{3/2}}{2\pi^{3/2}} \exp[-(m_X - \mu)/T], \quad (2.31)$$

where μ is the chemical potential of X .

Whether any long-lived dark matter (DM) particles are thermalized or not is determined by comparing the interaction rate (or the relaxation rate) Γ_{int} to the expansion rate of the Universe H , Eq. (2.8). In the RD phase, using Eq. (2.28) we obtain,

$$H = \begin{cases} \sqrt{\frac{\pi^2}{90M_{\text{P}}^2} g_* T^4} \simeq 0.136 \times 10^{-21} g_*^{1/2} T^2 \text{ MeV}^{-1} & \text{(RD)}, \\ \sqrt{\frac{1}{32\pi^{3/2} M_{\text{P}}^2} g_* m (mT)^{3/2} \exp[-(m - \mu)/T]} \\ \simeq 3.08 \times 10^{-26} \exp[-(m - \mu)/2T] g_*^{1/2} m^{5/4} T^{3/4} \text{ keV}^{-1} & \text{(MD)}. \end{cases} \quad (2.32)$$

When the interaction rate is much faster than the expansion time scale, if there are so many (energy and momentum changing) collisions before the scattering particles are apart by cosmic expansion,

$$\frac{\Gamma_{\text{int}}}{H} > 1, \quad (2.33)$$

the species are in thermal equilibrium. In the opposite case, they never reach thermal equilibrium. The temperature T_{dec} at the epoch $\Gamma_{\text{int}} = H$ is called the decoupling temperature of the particles. T_{dec} is slightly different from the freeze-out temperature T_{fr} , as shown in Fig. 2.4. We define T_{fr} such that the mass fraction of the particle stays constant below T_{fr} . Since they are very similar, we will not distinguish them in this book.

2.2.2. Decoupling temperature

In Fig. 2.4, we show the number density of X produced after inflation. In the red curve region, it is relativistic. When the temperature falls below $\sim 1/m_X$, its density is suppressed, when it is in equilibrium with radiation, by the exponential Boltzmann suppression factor as shown by the green curve. But below the decoupling temperature, the X particles lose the chance to scatter and its number density relative to radiation stays constant as shown by the blue curve.

The scattering rate depends on the nature of the leading interaction. If a $2 \rightarrow 2$ interaction (two particles going into two particles) with coupling g^2 is the leading

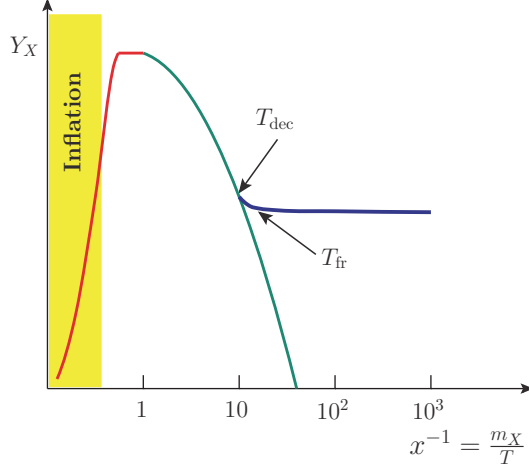


Fig. 2.4. Creation of massive particles X after inflation, for the chemical potential $\mu = 0$. Below the freeze-out temperature, the number density stays at a constant value. Y_X is the mass fraction of X relative to total baryonic mass.

one, a dimensional argument gives a rate at the cosmic temperature T in the RD phase as

$$\text{Dimension 4 interaction } (2 \rightarrow 2): \Gamma_{\text{int}} \approx \frac{g^4}{16\pi^2} E \sim \frac{g^4}{8\pi^2} T. \quad (2.34)$$

If the $2 \rightarrow 2$ interaction, involving fermions, has a nonrenormalizable coupling $1/M^n$, we obtain instead

$$\begin{aligned} \text{Dimension } n \text{ interaction } (2 \rightarrow 2): \Gamma_{\text{int}} &\approx \frac{1}{16\pi^2 M^{2n}} E^{2n+1} \\ &\sim \frac{1}{16\pi^2 M^{2n}} T^{2n+1}. \end{aligned} \quad (2.35)$$

So, for renormalizable interactions, we have

$$H \sim \frac{\pi g_*^{1/2} T^2 / \sqrt{30}}{\sqrt{3} M_{\text{P}}} \sim \frac{g^2}{16\pi^2} T \rightarrow T_{\text{dec}} \sim \frac{\alpha}{10} M_{\text{P}}, \quad (2.36)$$

where particles are in thermal equilibrium below T_{dec} for the case of dimension 4 interactions ($n = 0$). Taking $\alpha \sim \mathcal{O}(\frac{1}{20})$, the renormalizable interaction makes the species in thermal equilibrium below $T \approx 0.005 M_{\text{P}}$. For the dimension n interaction,

instead we have

$$\frac{\pi g_*^{1/2} T^2 / \sqrt{30}}{\sqrt{3} M_{\text{P}}} \sim \frac{1}{16\pi^2 M^{2n}} T^{2n+1} \quad (2.37)$$

$$\rightarrow T_{\text{dec}}^{2n-1} \sim \frac{16\pi^3 g_*^{1/2}}{\sqrt{90}} \left(\frac{M^{2n}}{M_{\text{P}}} \right), \quad (2.38)$$

where particles are thermally decoupled below T_{dec} , as shown in Fig. 2.4. Most WIMP candidates satisfy this relation which is a function of the mass M of the interaction mediator.

2.2.3. Interaction and decay rates

For the head-on collision, the scattering cross-section is given by

$$\begin{aligned} \sigma(X_1 + X_2 \rightarrow \dots) &= (2\pi)^{4-3n} \left(\frac{1}{|\mathbf{v}_1 - \mathbf{v}_2|} \right) \\ &\times \int \frac{d^3 \mathbf{p}'_1 \dots d^3 \mathbf{p}'_n}{2E_1 2E_2 2E'_1 \dots 2E'_n} |T_{X_1 X_2 \rightarrow n}|^2 \delta^4 \left(p_1 + p_2 - \sum_{i=1}^n p'_i \right), \end{aligned} \quad (2.39)$$

where the velocity difference $|\mathbf{v}_1 - \mathbf{v}_2|$ is the flux factor, the δ^4 factor is the total four-momentum conservation, $|T|^2$ is the invariant T -matrix squared and the integration is over all possible final momenta:

$$v_{\text{Moe}} = \sqrt{|\mathbf{v}_1 - \mathbf{v}_2|^2 - |\mathbf{v}_1 \times \mathbf{v}_2|^2}, \quad (2.40)$$

which is $\sqrt{(p_1 \cdot p_2)^2 - m_1^2 m_2^2} / E_1 E_2$ in the relativistic case [21] (see Fig. 2.5). Basically, it is the Lorentz contraction effect. With the same convention as in the

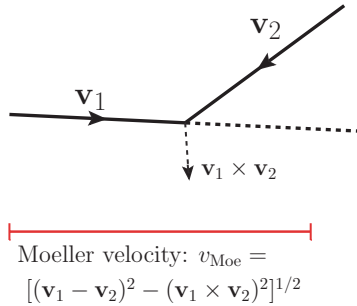


Fig. 2.5. The Moeller velocity.



Fig. 2.6. Production of a WIMP or E-WIMP by scattering and decay.

scattering case, the decay rate is given by

$$\Gamma(X \rightarrow \dots) = (2\pi)^{4-3n} \left(\frac{1}{|v_1 - v_2|} \right) \times \int \frac{d^3\mathbf{p}'_1 \cdots d^3\mathbf{p}'_n}{2E_X 2E'_1 \cdots 2E'_n} |T_{X \rightarrow n}|^2 \delta^4 \left(p_X - \sum_{i=1}^n p'_i \right). \quad (2.41)$$

The interaction Hamiltonian or Lagrangian enables one to calculate the T -matrix elements, which are extensively discussed in most quantum field theory books. The above formulas use the energy normalization of the one particle state, for example,

$$\langle 0 | \phi(x) | p \rangle = (2\pi)^3 2E \delta^3(\mathbf{p}) e^{ip \cdot x}. \quad (2.42)$$

Some particles interact much more weakly than the weak interaction rate, in which case WIMPs are called E-WIMPs. The E-WIMPs are not in thermal equilibrium, and they do not follow the equilibrium curve. But their creators X_1, X_2 , and X might have been in thermal equilibrium. This situation is depicted schematically in Fig. 2.11 [22]. WIMPs and E-WIMPs can be produced nonthermally by scattering or decay processes as shown in Fig. 2.6. To estimate the number density due to nonthermal production (NTP), we need the scattering rate for $X_1 + X_2 \rightarrow n$ particles and the decay width of a heavy particle $X \rightarrow n$ particles. In this short subsection, the formulas for these are summarized.

2.3. Cosmological nucleosynthesis

The best known example for the calculation of the decoupling temperature is the *decoupling temperature for nucleosynthesis* [23]. A review on BBN in modern particle theory, with weak neutral currents included, has been presented in [24] where a cosmic history up to below $T \simeq 10^{10}$ K has been concisely given. The basic atomic

number (Z) changing interactions in a nucleus (A, Z) are the weak interactions

$$p + e^- \leftrightarrow n + \nu_e, \quad (2.43)$$

$$p + \bar{\nu}_e \leftrightarrow n + e^+, \quad (2.44)$$

$$n \rightarrow p + e^- + \bar{\nu}_e. \quad (2.45)$$

For the β decay of radioactive nucleus, the neutron decay process (2.45) is the relevant one, producing antielectron-neutrino. In the early Universe with $T \approx 10^{11}$ K, the relevant $2 \leftrightarrow 2$ processes for $n = 2$ in Eq. (2.38) are Eqs. (2.43) and (2.44). We must also include Eq. (2.45). The ratio of neutron to proton at the equilibrium temperature is

$$\frac{n}{p} \simeq e^{-\Delta m/T}. \quad (2.46)$$

The neutron/proton ratio we observe today is basically this primordial number calculated at the time of ν_e and $\bar{\nu}_e$ decoupling by the charged current weak interaction with proton and neutron, presented in Eqs. (2.43), (2.44), and (2.45).

A succinct nuclear reaction history up and below $T \simeq 10^{10}$ K is the following [24]:

- 3×10^{10} K $< T < 10^{11}$ K (10^{-2} s $< t < 0.1$ s): With kinetic energies of O(10 MeV), comparable numbers of $e^\pm$, ν_i , $\bar{\nu}_i$, and photon were in thermal equilibrium with a tiny amount of baryons p and n . The weak interaction is strong enough to keep them in the thermal equilibrium. The neutral current interaction [25] $\nu_e + \bar{\nu}_e \leftrightarrow \nu_i + \bar{\nu}_i$ made muonic and tau neutrinos were as copious as electron neutrinos, which contributed in the determination of the neutron/proton ratio n/p at decoupling temperature T_{dec} . The g_* for energy density ρ of relativistic particles at this time with three neutrino species is

$$g_* = \frac{43}{4} = 2 \left|_{\gamma} + 3 \frac{7}{8} \right|_{\nu} + 3 \frac{7}{8} \left|_{\bar{\nu}} + \frac{7}{4} \right|_{e^-} + \frac{7}{4} \left|_{e^+} \right|. \quad (2.47)$$

- $T \approx 3 \times 10^{10}$ K ($t \approx 0.1$ s): The neutral current interactions, i.e., $\nu_\mu, \bar{\nu}_\mu, \nu_\tau$, and $\bar{\nu}_\tau$, are decoupled. At this epoch, T_{ν_μ} is calculated to be about a few MeV.
- $T \approx 10^{10}$ K ($t \approx 1$ s): The charged current interactions become decoupled. The g_* at this time with one neutrino species is

$$g_* = \frac{29}{4} = 2 \left|_{\gamma} + \frac{7}{8} \right|_{\nu_e} + \frac{7}{8} \left|_{\bar{\nu}_e} + \frac{7}{4} \right|_{e^-} + \frac{7}{4} \left|_{e^+} \right|, \quad (2.48)$$

where we do not count $\bar{\nu}_\mu, \nu_\mu, \bar{\nu}_\tau$, and ν_τ . At this epoch, T_{ν_e} is calculated to be about 0.8 MeV.

- $T \approx 3 \times 10^9 \text{ K}$ ($t \approx 10 \text{ s}$): The process $p + n \leftrightarrow D + \gamma$ keeps the manufactured deuteron in thermal equilibrium with proton and neutron, by energetic γ rays in the Boltzmann spectrum. So, the deuteron number is determined by the equilibrium condition. Still, the ratio n/p has been determined except for a small decrease by the free neutron decaying to proton plus $(e + \bar{\nu}_e)$. Thus, the ratio n/p keeps decreasing with lifetime of 880 s. This period is called the deuteron bottleneck.
- $T \approx 10^9 \text{ K}$ ($t \approx 10^2 \text{ s}$): Temperature is low enough such that the process $p + n \leftrightarrow D + \gamma$ is out of equilibrium. It can be called the deuteron decoupling. Now, all neutrons living in the deuteron nuclei are stable. Most of these deuterons end up as helium nuclei and the ratio $n/p \simeq 1/7$ gives the primordial abundance of ^4He . Still, a small fraction remains as deuterons.
- $T \approx 4 \times 10^8 \text{ K}$ ($t \approx 10^3 \text{ s}$): At this time, more light nuclei such as ^3He and ^7Li are made by nuclear processes. This time scale is considered to be the end of primordial nucleosynthesis.

For the BBN, two decoupling temperatures appear. There is the decoupling temperature T_{ν_e} by the charged current interaction. The decoupling temperature T_{ν_μ} for the second and third family neutrinos ($\nu_\mu, \nu_\tau, \bar{\nu}_\mu$ and $\bar{\nu}_\tau$) is calculated via the neutral current cross-section with nucleons. For example, the center of momentum scattering cross-section for the process,

$$\nu_\mu(E, \mathbf{p}) + \bar{\nu}_\mu(E, -\mathbf{p}) \rightarrow \nu_\tau(E, \mathbf{p}') + \bar{\nu}_\tau(E, -\mathbf{p}'), \quad (2.49)$$

is given by

$$\sigma_{\text{NC}} = \frac{G_F^2}{3\pi} \cos^2 \theta_W E^2, \quad (2.50)$$

where θ_W is the weak mixing angle in the SM, $\cos^2 \theta_W \simeq 0.77$ [26]. To obtain the rate of interaction in one Hubble time, we use the number density of neutrinos given in Eq. (2.30).

The decoupling temperature T_{ν_e} for the first family of neutrinos is calculated via the charged current cross-section. The relevant charged current interaction is of the $(V - A) \cdot (V - A)$ form,

$$\mathcal{H}_{\text{int}} = \frac{G_F}{\sqrt{2}} \bar{n} \gamma^\mu (1 + \gamma_5) p \bar{\nu}_e \gamma_\mu (1 + \gamma_5) e + \text{h.c.}, \quad (2.51)$$

where

$$G_F \simeq 1.16639 \times 10^{-5} \text{ GeV}. \quad (2.52)$$

For the electron energy $E_e < 10 \text{ MeV}$ in the RD universe, the cross-section for the process

$$p(E_p, \mathbf{k}) + e^-(E, -\mathbf{k}) \leftrightarrow n(E_n, \mathbf{k}') + \nu_e(E_\nu, -\mathbf{k}') \quad (2.53)$$

is given by

$$\sigma_{CC} = (1 + 3g_A^2) G_F^2 \cos \theta_C \frac{q^2}{2\pi} \quad \text{with } (1 + 3g_A^2) = (1 + g_A)^2, \quad (2.54)$$

as presented in Section 2.6.5. Here, $g_A \simeq 1.26$ and $\sin \theta_C \simeq 0.2253$ [27]. Let the overall constant be A , i.e.,

$$A = \frac{G_F^2 (1 + 3g_A^2) \cos^2 \theta_C}{2\pi^3}. \quad (2.55)$$

For the ratio of n/p , the constant A drops out, but in the calculation of T_{dec} by $\Gamma \simeq H$, we must keep the interaction strength. The same constant A also appears in the neutron decay rate

$$\tau_n^{-1} = \Gamma_{n \rightarrow pe\bar{\nu}_e} = A m_e^5 \int_1^\epsilon d\epsilon \epsilon(\epsilon - q)^2 \sqrt{\epsilon^2 - 1} \simeq 1.636 A m_e^5, \quad (2.56)$$

where dimensionless variables are in units of m_e : $\epsilon = E_e/m_e$ and $q = Q/m_e$ with Q -value in the decay. The mean lifetime of neutron $\tau_n (= \tau_{1/2}/\ln(2))$ is about 15 minutes, 880.0 ± 0.9 s [27] which enters into the determination of the decoupling temperature of free neutron in the cosmos.

The equilibrium condition takes into account all these processes folded over the appropriate phase spaces of incoming particles. The incoming particle phase space is limited by the Q value in the process. For the forward direction of Eq. (2.43), $Q = E_e - E_\nu$ which adds up to proton energy to become neutron energy. For (2.38), we use $M = v_{\text{ew}} \simeq 246$ GeV.

For the $\rightarrow$ direction in Eq. (2.43), therefore, we fold over the distribution of phase space for $T < 10^{11}$ K as

$$\Gamma(p + e^- \rightarrow n + \nu_e) = A \int_{-\infty}^{+\infty} dq \frac{q^2 (Q + q)^2 \sqrt{1 - \frac{m_e^2}{(Q+q)^2}}}{(1 + e^{-q/k_B T_\nu})(1 + e^{(Q+q)/k_B T})}, \quad (2.57)$$

excluding the gap $q = [-Q - m_e, -Q + m_e]$ in the integration over dq .

In the high temperature and low temperature limits, the scattering rate in the Universe is given by [8], assuming relativistic e hitting on p at rest,

$$\Gamma(pe \rightarrow n\nu_e) = \begin{cases} \tau_n^{-1} \left(\frac{T}{m_e} \right)^3 e^{-Q/T}, & T \ll Q, m_e, \\ \frac{7}{60} \pi (1 + 3g_A^2) G_F^2 T^5 \simeq 2.62 G_F^2 T^5, & T \gg Q, m_e. \end{cases} \quad (2.58)$$

For the Hubble rate in the RD phase, we use $H \simeq \sqrt{\pi^2 g_*/90} T^2/M_{\text{P}} \simeq 0.294 T^2/M_{\text{P}}$. Here, we used $g_* = \sqrt{29/4}$ since $\bar{\nu}_\mu, \nu_\mu, \bar{\nu}_\tau, \nu_\tau$ are already decoupled

at $T \simeq 10^{10}$ K. Thus, the second equation of (2.58) gives, $G_F^2 T_{\nu_e}^5 \approx 1.09 \frac{T_{\nu_e}^2}{M_P}$,

$$T_{\nu_e} \approx \left(\frac{0.294}{1.16^2 \times 10^{-10} \times 2.43 \times 10^{18}} \right)^{1/3} \text{ GeV} \rightarrow T_{\nu_e} \approx 0.96 \text{ MeV}. \quad (2.59)$$

This preliminary number should be more accurately calculated considering that e is not fully relativistic for the flux factor in Eq. (2.39) and its number density is not $\propto T^3$ but $\propto T^3 e^{-|p|e/T}$, and also by adding the contributions of other neutrinos ($\bar{\nu}_\mu, \nu_\mu, \bar{\nu}_\tau, \nu_\tau$) whose temperature is lower than that of ν_e . These considerations further lower the temperature down to 0.72 MeV.

Example 2.1 (Photon and neutrino temperatures). The neutrino/photon temperature ratio uses the fact that photons are reheated after e^+e^- annihilation below 0.5 MeV. The ν_e energy density is fixed below $T_\nu \simeq 0.72$ MeV as $\propto \frac{7}{8} T_\nu^4$. The g_* factor of e^+e^- is $\frac{7}{4} + \frac{7}{4} = \frac{7}{2}$. The energy of e^+ and e^- goes into that of photon. Thus, the photon energy density is increased to $\propto (2 + \frac{7}{2}) T_\nu^4 = \frac{11}{2} T_\nu^4$ which is interpreted as $\propto 2T_\gamma^4$. Thus, we obtain the relation $T_\gamma = (11/4)^{1/4} T_\nu \simeq 1.29 T_\nu$.

The decoupling temperature also depends on the presence of relativistic particles around the time of decoupling. The above temperature is based on the assumption of three neutrino species. Leptons in the SM of Table 1.1 are

$$\begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, e_R, \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}_L, \mu_R, \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}_L, \tau_R, \quad (2.60)$$

where we inserted only three families. Once the decoupling temperature is known, the neutron/proton ratio is calculated as

$$\left. \frac{n}{p} \right|_{T_{\nu_e}} \simeq e^{-\Delta m/T_{\nu_e}}, \quad \Delta m = m_n - m_p \simeq 1.293 \text{ MeV}. \quad (2.61)$$

One can define Y_i as the mass fraction of nucleus i compared to the total atom mass density,

$$Y_i = \frac{\rho_i}{\rho_{\text{atoms}}}. \quad (2.62)$$

But, usually it is used only for ${}^4\text{He}$. Moreover, Y_p (instead of $Y_{{}^4\text{He}}$ in this case), the mass fraction of the observed primordial helium, is [28]

$$Y_p \equiv \frac{\rho_{{}^4\text{He}}}{\rho_b} = \frac{2(n/p)}{1 + n/p} \simeq 0.25, \quad (2.63)$$

which requires the neutron/proton ratio $n/p \simeq \frac{1}{7}$. Note that $n/p \simeq \frac{1}{6}$ at $T \simeq 0.72$ MeV, which is reduced to $\frac{1}{7}$ by occasional weak interactions (eventually dominated by free neutron decays as commented before).

The success of the BBN calculation on the primordial ^4He abundance allowed us to scrutinize the Universe at the cosmic time at 1 s. Firstly, it predicts that the number of light neutrinos is not much larger than 3 [24, 25].⁵ If there were more than three effective neutrinos, then the decoupling temperature goes up, the ratio n/p goes up, and the prediction of ^4He abundance goes up. Thus, the effective number of neutrinos affects the ^4He abundance [24].

At the cosmic time 1 s, the Universe temperature is of order MeV where nuclear physics plays the dominant role. The primordial ^4He abundance depends on the single nucleon interactions of Eqs. (2.43), (2.44), and (2.56), and the predicted abundance is given by Eq. (2.61) since all neutrons manufactured mostly end up as ^4He . The next simplest nuclear reaction is $n + p \leftrightarrow D + \gamma$. Deuterium synthesized in this way finds itself destroyed by energetic γ rays (the CMB blueshifted to average photon energies $E_\gamma \sim 3T_\gamma \gtrsim \text{few MeV}$) in the background of CMB photons. Deuterium is thus photo-dissociated, and BBN of D still continues, and T_γ falls down to $\sim 80 \text{ keV}$ [25]. Until this time ^4He has not been manufactured as predicted because in the nuclear reactions to make up ^4He the interim material D is needed. This period from 0.8 MeV down to 80 keV is the deuterium bottleneck. The end of deuterium bottleneck was at the cosmic time 180 s which was called “The First Three minutes” by Weinberg [30]. More nuclear physics reaction chains are needed to produce heavier elements, ^3He and ^7Li . With all possible nuclear processes, the Universe has manufactured the primordial light elements ^4He , D, ^3He , and ^7Li , but not effective in making heavier elements such as C, O, etc. The cosmic BBN processes are coded in Ref. [31], which are presented in the PDG book [28] as shown in Fig. 2.7. The yellow margins in the vertical direction are the observed 95% CL bounds. Helium is also copiously produced during star evolution, which is not included in Fig. 2.7. Thus, the primordial BBN production is firm with a small error bar [25],

$$Y_p = 0.2483 \pm 0.0005 + 0.0016(\eta_{10} - 6). \quad (2.64)$$

Other light elements are much rarer,

$$\text{D}/\text{H} = (2.67 \pm 0.08) \times 10^{-5} \left(\frac{6}{\eta_{10}} \right)^{1.6}, \quad (2.65)$$

$$^3\text{He}/\text{H} = (1.06 \pm 0.032) \times 10^{-5} \left(\frac{6}{\eta_{10}} \right)^{0.6}, \quad (2.66)$$

$$^7\text{Li}/\text{H} = (4.30 \pm 0.43) \times 10^{-10} \left(\frac{6}{\eta_{10}} \right)^2, \quad (2.67)$$

⁵This observation [29] was made before the particle physics constraint from the LEP experiments was available.

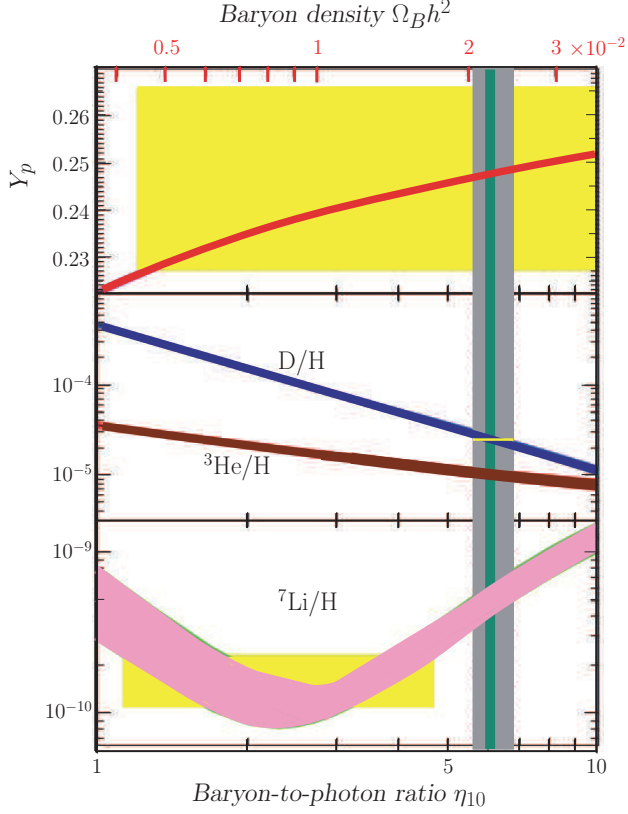


Fig. 2.7. Primordial abundances (95% CL) of ${}^4\text{He}$, D, ${}^3\text{He}$, and ${}^7\text{Li}$ vs. $\Omega_B h^2$ and η_{10} , presented in the PDG book [28]. The observed limits are shown as yellow bands. The helium abundance has a large uncertainty while the deuterium bound is most constraining. Wide curved bands are the prediction from the BBN calculation. The vertical green band is from the CMB measure of the baryon density and the wider gray band is the concordance range with BBN deuterium (95% CL).

where

$$\eta_{10} \equiv 10^{10} \left(\frac{n_B}{n_\gamma} \right). \quad (2.68)$$

Comparing the BBN model and the yellow bands, the deuterium abundance is most constraining. The narrow vertical green band is from the CMB measure of the baryon density, which is compared to the BBN prediction, presented as the gray band. The ${}^7\text{Li}$ production in the BBN also has a narrow band, viz. the ${}^7\text{Li}/\text{H}$ scale is different from that of D/H. At present, the ${}^7\text{Li}/\text{H}$ band is out of the CMB measure of $\Omega_B h^2$. So, there exist some attempts to manufacture ${}^7\text{Li}$ as in Ref. [32].

In Fig. 2.7, the CMB data on η_{10} is at a very narrow band, 6.11 ± 0.20 i.e., $n_B/n_\gamma \simeq 0.61 \times 10^{-9}$, due to the temperature fluctuations observed at Planck [33].

It gives $\Omega_B h^2 = 0.0223 \pm 0.0007$ [25]. This baryon density is the one shown as atoms in Fig. 1.2.

2.4. Baryon number in the Universe

The baryon number density $n_B/n_\gamma \simeq 6.1 \times 10^{-10}$ is one of the most accurately determined quantity in the precision cosmology. At the cosmic temperature above 1 GeV, numbers of baryons and antibaryons must be comparable to that of photons. But the present value of n_B/n_γ is extremely small $O(10^{-9})$, implying a scenario that the Universe has started with the net baryon number almost zero before BBN,

$$\Delta B \equiv \frac{n_B - n_{\bar{B}}}{n_\gamma} \simeq 0, \quad \text{at } t \ll 1 \text{ s.} \quad (2.69)$$

If indeed the Universe started with $\Delta B = 0$ at the time of CDM density fixed, our Galaxy happens to be a baryon galaxy while some other galaxy must be made of antibaryons. Since the probability of separating astronomical number of protons from another astronomical number of antiprotons is completely negligible and the observed n_B is nonzero (even though tiny), the Universe must have evolved to one with $\Delta B \simeq 10^{-9}$ much earlier than the BBN time.

This poses a question, “How can one generate a nonzero net baryon number starting from an initial $\Delta B = 0$ Universe?” This is the so-called *baryogenesis* problem. Three physical conditions are listed for baryogenesis by Sakharov [34]:

- (i) There must have been interactions with microscopic violation of baryon number.
- (ii) These interactions simultaneously violate C and CP symmetries.
- (iii) These processes occurred out of thermal equilibrium.

These physical conditions seem obvious. To create a nonzero ΔB out of $\Delta B = 0$, one needs some baryon number violating interactions. Of course, the difference of particles and antiparticles must be created, which means the existence of C violation. In case C is violated, consider the opposite point of $\mathbf{x}$ ($\mathbf{x} \rightarrow -\mathbf{x}$), obtained by P operation. Consider the number of particles ΔB at the red clover point of Fig. 2.8. If CP is conserved, the P operated point (the black clover) should have exactly the same number of antiparticles. Thus, in CP conserving theories, the particle number in the first octant is the same as the antiparticle number in the skyblue octant, and there will be no net ΔB generated,

$$\int d^3\mathbf{x} n_B - \int d^3\mathbf{x} \bar{n}_B = 0. \quad (2.70)$$

Thus, there will be no net baryon number generation if CP is conserved. Finally, if the process were in thermal equilibrium, the rate $A + B \rightarrow C + D$, producing ΔB , is equal to the rate $C + D \rightarrow A + B$, producing $-\Delta B$.

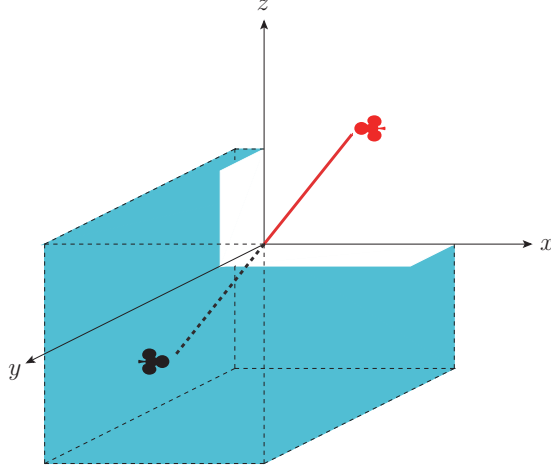


Fig. 2.8. The CP operation on $\clubsuit$ in the first octant with coordinate (a, b, c) . It goes into the skyblue box as $\clubsuit$ with coordinate $(-a, -b, -c)$.

Example 2.2 (C violation needed). One can show the need for C violation in another way. Firstly, to have a nonzero ΔB , we need T violation. At the red clover point of Fig. 2.8, let us calculate baryons moving forward/backward in time. The ratio is the number of baryons over the number of antibaryons. Second, integrate over solid angles. At the black clover point, if C is not broken, then ΔB is minus that of red clover point, because $P = -1$ is multiplied. Then, integration over the solid angle gives $\Delta B = 0$. Therefore, the needed T violation in the $\Delta B \neq 0$ processes must accompany the C violation also.

But around the late 1960s, $\Delta B \neq 0$ interactions were hard to figure out, when the fundamental interactions even just above the scale relevant for nuclear physics were not known. After the discoveries of weak neutral current and asymptotic freedom, the SM has emerged as the model describing physics up to 100 GeV scale. But, the baryon number is not violated in the SM. The baryon number violating interaction appeared in the grand unification theories (GUTs) [35, 36] unifying strong, electromagnetic, and weak forces of the SM. Then, proton decay has been considered to be the most important prediction of GUTs [37]. The $\Delta B (= B_{\text{initial}} - B_{\text{final}})$ nonzero processes in GUTs have been appreciated in 1978 [38] since the BBN was firmly accepted after 1977 [30, 39]. Departures from thermal equilibrium occur in an expanding Universe, possibly satisfying the third condition. A significant $\Delta B \neq 0$ is difficult to be realized by scattering processes at a GUT temperature since the scattering processes of ordinary (i.e., effectively massless) fermions have no mass threshold as pointed out by Toussaint, Treiman, Wilczek, and Zee [40]. But, it was shown that the decay of a heavy X could produce an appropriate ΔB as the temperature T falls below the mass M_X [41]. Then, this does not belong to the class of thermal production but to the class of NTP of ΔB . Furthermore, if the decay

products are the SM fermions where the CP phase is provided by the CKM matrix, a calculation shows $\Delta B \approx 10^{-18}$ [42]. Thus, a GUT scenario for ΔB generation has moved for the decaying scalar case: X decaying to particles carrying nonzero baryon numbers.

This GUT-scale generation of ΔB went into another twist because of the QCD instanton process, violating the baryon number [43]. Applying this to SU(2) weak sphaleron processes, one expects that baryon number (B) violation, but with baryon minus lepton number ($B - L$) conservation, occurred at the electroweak phase transition in the evolving Universe [44]. Even if ΔB was generated at a GUT scale, it might have been erased. Since $B - L$ is conserved, the generation of lepton number at a high energy scale, of which some is converted to the baryon number during the electroweak phase transition, was suggested [45]. This is the so-called *leptogenesis*. Yet, a new mechanism for baryogenesis above electroweak scale, innocent of the electroweak phase transition, has also been suggested [46]. There is also another mechanism where an evolving scalar(s) generates the baryon number, which is called the Affleck–Dine mechanism [47]. Among these, the leptogenesis mechanism has received most interest, and it will be discussed more in Chapter 8.

2.5. Thermal WIMP production in the Universe

WIMPs as thermal relics remain as the most scrutinized possibility for DM. It is because the scattering cross-section is of the order of the weak interaction cross-section we have the letter “W” in WIMP. If the DM is a WIMP, it can be discovered as the effects of weak-force mediator W and Z have been observed. In Chapter 1, candidates for DM particles are required to be

- (1) nonbaryonic,
 - (2) stable (or at least extremely long lived), and
 - (3) nonrelativistic at the time of CDM density fixed era.
- (2.71)

In the early Universe, WIMPs (denoted by X) are assumed to be in thermal equilibrium. The WIMP number density n_X evolves according to the Boltzmann equation,

$$\frac{dn_X}{dt} = -3Hn_X - \langle \sigma_{\text{ann}} v \rangle (n_X^2 - n_{\text{eq}}^2), \quad (2.72)$$

where σ_{ann} is the annihilation cross-section for X to disappear and $\langle \sigma_{\text{ann}} v \rangle$ is the thermally averaged value with the WIMP velocity v . An approximate solution of Eq. (2.72) for large t is $n_X = n_{\text{eq}}$ since Hn_X is negligible for large t . Here n_{eq} is the number density below T_{dec} of X . It has been shown in Fig. 2.4.

2.5.1. Heavy neutrino

The first example calculation of cosmic WIMP scattering rate is due to Hut [48] and Lee and Weinberg [49]. In addition to the three families of leptons of (2.60), suppose that there is the fourth lepton family,

$$\begin{pmatrix} N \\ L \end{pmatrix}_R, \quad \begin{matrix} N_R, \\ L_R. \end{matrix} \quad (2.73)$$

Ref. [49] gave a ballpark number $\langle\sigma v\rangle$ as $G_F^2 m_N^2 N_{\text{ann}}/2\pi$, where N_{ann} is the number of the annihilation channel. For guidance, we can check that N_{ann} for the addition of (2.73) is 33 for $2\text{ GeV} \lesssim m_N \lesssim 5\text{ GeV}$,

$$3_{\text{families}} \left(1 \Big|_{\nu_e} + 2 \Big|_e \right) + 2_{\text{families}} \cdot 3_{\text{colors}} \left(2 \Big|_u + 2 \Big|_d \right) = 33, \quad (2.74)$$

where we counted three colors and considered only u, d, s , and c quarks.

Dirac neutrino

In the expanding Universe with the background radiation, this cross-section is folded over the Boltzmann distribution of the incoming light leptons with energy k . At the cosmic time with temperature T , the interaction rate is proportional to T^5 . The result of this folding gives the current energy density of N , which is shown in Fig. 2.9. Note that, for heavier neutrino mass in the GeV region, the abundance goes down as the mass goes up. This is because we fixed the interaction coefficient as G_F . In other words, we worked in the regime where the neutrino mass is lighter than the force mediator $W^\pm$. Then, we found that the heavier the neutrino, the lower the abundance.

However, this simple model is excluded already long time ago. It is because N carries nontrivial SM gauge quantum numbers.

Majorana neutrino

If the heavy neutrino is treated as a Majorana particle, one has to find out the changes in the cross-section calculation due to the Majorana nature. The meaningful change comes from the higher k^2 dependence of the cross-section, leading to the interaction rate proportional to T^7 . In fact, this raises the decoupling temperature a bit and also raises the abundance. It is shown as the red curve in Fig. 2.9. There are also changes in the number of initial spin average and also the inverse propagator of the Majorana neutrino, which actually cancel each other.

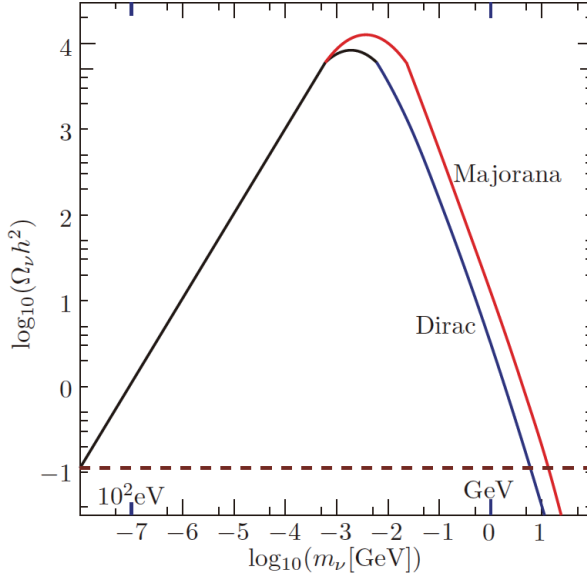


Fig. 2.9. A sketch of neutrino abundance plot. Light neutrinos are on the left-hand side (LHS) of the curve and heavy neutrinos are on the RHS of the curve. Majorana neutrinos have a bit more abundance compared to the same mass Dirac neutrino.

2.5.2. Forces for weakly interacting massive particles

The heavy neutrino discussed in Section 2.5.1 belongs to the class of weakly interaction massive particles (WIMPs). Since the heavy neutrino possibility seems already ruled out, the currently mentioned WIMP implies a hypothetical particle possessing a nonrenormalizable interaction strength of the order of G_F .⁶ It means that the mass of the *new* interaction mediator is comparable to the W -boson mass with the couplings of $O(0.01 - 1)$. Within this scheme, many hypotheses for the mediators of the needed interactions have been suggested. These mediators can be bosons or fermions. Possible force mediators are

- Particles in the SUSY scenario: Some particles in the SUSY extension of the SM, coupling to a hypothetical WIMP, are the needed force mediators. If the gauge hierarchy problem is solved by TeV-scale SUSY, the mediators are in the TeV range. This TeV range stands for “W” of WIMP.
- New Yukawa couplings: In the SM, a WIMP as an SM singlet is introduced. Then, the only possible interaction with the SM particles is by Yukawa couplings. Due to a vast range of allowed Yukawa couplings, the mediator mass can have a wide range.

⁶It was commented below Eq. (2.38) that nonrenormalizable interactions are the needed ones.

- Electroweak couplings: In the SM, a WIMP can be a nonsinglet member of the SM gauge group. Then, the dominant interaction of WIMP with the SM particles is by $W^\pm$ and Z of the SM. We already discussed a heavy neutrino N belonging to this case. So, possible models should evade the problems posed in the heavy neutrino case.
- New gauge boson(s): The WIMP possesses new gauge quantum numbers, and the needed interactions are by the corresponding gauge interactions. The new gauge boson mass must be cooked to be in the TeV range.

2.5.3. *WIMP relic density*

The energy density equation in the expanding Universe, Eq. (2.7), becomes the number density equation for a WIMP (with $p = 0$) if its number density n remains constant in the comoving volume. In the thermal bath, the equilibrium conditions determine the WIMP decoupling temperature as presented in Fig. 2.4. In this figure, the number density in the comoving volume changes above T_{dec} due to interactions. To calculate the decoupling temperature, thus, we consider the evolution equation of the phase space distribution function $f(\mathbf{x}, \mathbf{v}, t)$ above T_{dec} , satisfying the Boltzmann equation [8],

$$\hat{\mathbf{L}}[f] = \mathbf{C}[f], \quad (2.75)$$

where $\hat{\mathbf{L}}$ is the Liouville operator, and $\mathbf{C}$ is the collision operator. The nonrelativistic form of $\hat{\mathbf{L}}$ is

$$\hat{\mathbf{L}} = \frac{d}{dt} + \frac{d\mathbf{x}}{dt} \cdot \vec{\nabla}_x + \frac{d\mathbf{v}}{dt} \cdot \vec{\nabla}_v = \frac{d}{dt} + \frac{d\mathbf{x}}{dt} \cdot \vec{\nabla}_x + \frac{1}{m} \frac{d\mathbf{p}}{dt} \cdot \vec{\nabla}_v. \quad (2.76)$$

The covariant generalization of the Liouville operator is

$$\hat{\mathbf{L}} = -p^\alpha \frac{\partial}{\partial x^\alpha} + \Gamma_{\beta\gamma}^\alpha p^\beta p^\gamma \frac{\partial}{\partial p^\alpha}. \quad (2.77)$$

In a homogeneous and isotropic FLRW Universe, $f(\mathbf{x}, \mathbf{p}, t)$ becomes $f(|\mathbf{p}|, t) = f(E, t)$, and also $\hat{\mathbf{L}}$ simplifies to

$$\hat{\mathbf{L}} = E \frac{\partial}{\partial t} - \frac{\dot{R}}{R} |\mathbf{p}|^2 \frac{\partial}{\partial E}. \quad (2.78)$$

Then, the WIMP number density n that we are interested in becomes

$$n(t) = \sum_{\text{spins}} \int \frac{g d^3p}{(2\pi)^3} f(E, t), \quad (2.79)$$

where g is the spin degrees of freedom, describing Fermi–Dirac or Bose–Einstein statistics. So, $\sum_{\text{spins}}$ must be taken into account. Let us apply the Liouville operator

(2.78), after the integration over the phase space, i.e., $[2d^3p/(2\pi^3)2E]f$. Then, the time evolution of number density is given by

$$\frac{d}{dt}n + 3Hn = 2 \left[\int \frac{d^3p}{(2\pi)^3 2E} \mathbf{C}[n_{\text{others}}] n \right]. \quad (2.80)$$

Example 2.3 (The Hubble expansion factor in the number density). Then, the second term of (2.78) gives

$$\begin{aligned} & - \int \frac{d\Omega |\mathbf{p}|^2 dp}{(2\pi)^3 E} |\mathbf{p}|^2 \frac{\partial}{\partial E} f(E, t) = - \int \frac{d\Omega dE}{(2\pi)^3} \frac{\partial}{\partial E} |\mathbf{p}|^3 f(E, t) \\ & \quad + \int f(E, t) \frac{d\Omega dp}{(2\pi)^3} \frac{\partial}{\partial E} |\mathbf{p}|^{3/2} \\ & = - \int \frac{d\Omega dE}{(2\pi)^3} \frac{\partial}{\partial E} |\mathbf{p}|^3 f(E, t) + \int f(E, t) \frac{d\Omega dE}{(2\pi)^3} 3E(E^2 - m^2)^{1/2} \\ & = - \int \frac{d\Omega dE}{(2\pi)^3} \frac{\partial}{\partial E} |\mathbf{p}|^3 f(E, t) + 3 \int f(E, t) \frac{d^3p}{(2\pi)^3} \\ & = - \frac{1}{2\pi^2} |\mathbf{p}|^3 f(E, t) \Big|_0^{|\mathbf{p}|_{\max}} + 3 \int f(E, t) \frac{d^3p}{(2\pi)^3} \\ & \rightarrow 3 \int f(E, t) \frac{d^3p}{(2\pi)^3}, \end{aligned} \quad (2.81)$$

to which the $|\mathbf{p}|$ independent $\dot{R}/R$ is multiplied, and the last line is given in the nonrelativistic regime. Therefore, in the nonrelativistic regime, we obtain the H dependence of the number density in the expanding Universe,

$$\frac{d}{dt}n + 3Hn = 2 \left[\int \frac{d^3p}{(2\pi)^3 2E} \mathbf{C}[n_{\text{others}}] n \right].$$

In Eq. (2.80), the RHS is given by the cross-section for the process

$$a + b \rightarrow c + d + \dots. \quad (2.82)$$

In the cross-section formula, if the two-body collision is not head-on, the flux factor $|\mathbf{v}_a - \mathbf{v}_b|$ in the denominator in Eq. (2.39) should be replaced by the Moeller velocity factor v_{Moe} given in Eq. (2.40). This means that the average of $\langle \sigma v \rangle$ should use v_{Moe} , which has been given explicitly in Ref. [50]. In calculating this rate average, $\langle \sigma v_{\text{Moe}} \rangle$, we average over the cross-section of a on the target particle b , considering the fluxes, which is for a specific incoming spin states. However, in the thermal average, we do not consider specific initial spin states, but consider all possible spins in the thermal background. Therefore, we just sum over the initial spins. This introduces n_b in the formula (2.80). For the outgoing particles, $c, d, \dots$, we have already integrated over the phase space. To a , the target b looks like approaching him with v_{Moe} , and the

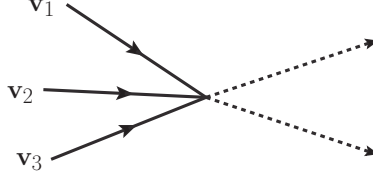


Fig. 2.10. Three incoming particles.

flux factor is $n_b v_{\text{Moe}}$ with dimension $[\text{cm}^{-2} \text{s}^{-1}]$. Thus, the cross-section formula (which has v_{Moe} in the denominator implicitly) is multiplied by v_{Moe} in the thermal average $\langle \sigma v_{\text{Moe}} \rangle$. So, the thermal average does not seem to be distinguishing the initial and final particles. Finally, the RHS of Eq. (2.80), for $n = n_a$ on the LHS, can be written as [50]

$$- \int \sigma v_{\text{Moe}} (dn_a dn_b - dn_{a,\text{eq}} dn_{b,\text{eq}}), \quad (2.83)$$

where the final spin sum and initial spin average have to be taken into account carefully.

Example 2.4 (Three-body initial states). If three particles are incoming, as shown in Fig. 2.10, v_{Moe} should take into account three incoming velocities, but in the thermal average, it should cancel out in the same way that has been explained above. The generalized v_{Moe} is

$$(|\mathbf{v}_1 - \mathbf{v}_2| - |\mathbf{v}_1 \times \mathbf{v}_2|) \cdot (|\mathbf{v}_1 - \mathbf{v}_3| - |\mathbf{v}_1 \times \mathbf{v}_3|)$$

because particle 1 considers both the fluxes of 2 and 3.

If one incoming particle is relativistic, σv_{Moe} has the same order as that of just σc and the thermal bath of relativistic particles b has the density proportional to T^3 . Therefore, the RHS of Eq. (2.80) is proportional to $\sigma T^3 n_a$. This is the condition $H \simeq \Gamma$ used to find out T_{dec} in Section 2.3. The schematic behavior from Eq. (2.80) is shown in Fig. 2.4.

Since the thermal average does not distinguish the initial and final states, the rate for a process (2.82) and its inverse process has the same thermal average

$$\begin{aligned} & \sum_{\text{all spins}} \int \frac{d^3 p_a}{(2\pi^3) 2E_a} \frac{d^3 p_b}{(2\pi^3) 2E_b} \frac{d^3 p_c}{(2\pi^3) 2E_c} \frac{d^3 p_d}{(2\pi^3) 2E_d} (\dots) \\ & \times |T_{\rightarrow} \text{ or } T_{\leftarrow}|^2 \delta^{(4)}(p_a + p_b - p_c - \dots), \end{aligned} \quad (2.84)$$

where $\rightarrow$ and $\leftarrow$ are for the forward and backward processes, respectively. Since $\sum_{\text{all spins}} |T_{\rightarrow}|^2 = \sum_{\text{all spins}} |T_{\leftarrow}|^2$, we obtain the so-called detailed balance in statistical equilibria. Consequently, the decoupling temperature, averaging over $\langle \sigma v \rangle$, does not depend on the velocity used, v or v_{Moe} . Even if the detailed balance does

not depend on the velocity used, the cross-section σ depends on the velocity and the Moeller velocity is the relevant one to calculate the cross-section. This result affects the calculation of WIMP detection rate.

Finally, the incoming particles a and b , on the RHS of (2.83) producing WIMP, must have thermal distribution before the decoupling is reached. So, we take the thermal average of σv_{Moe} ,

$$\langle \sigma v_{\text{Moe}} \rangle = \frac{\int \sigma v_{\text{Moe}} e^{-E_a/T} e^{-E_b/T} d^3 p_a d^3 p_b}{\int e^{-E_a/T} e^{-E_b/T} d^3 p_a d^3 p_b}. \quad (2.85)$$

We noted before that

- $\langle \sigma v_{\text{Moe}} \rangle$ is Lorentz invariant, and
- v_{Moe} becomes $|v_a - v_b|$ for the head-on collision.

The simple description presented above on thermal WIMP production has three exceptions as discussed by Griest and Seckel [51],

- (1) resonances;
- (2) thresholds;
- (3) co-annihilations.

These exceptions have to be taken into account in calculating the detection rate, and hence constraining models. These points will be discussed more in Chapter 9.

2.6. Nonthermal production

Thermal production of a candidate CDM particle is sketched in Fig. 2.4, which describes Eq. (2.80). Any other expression for the number density is called nonthermal production. WIMPs can be produced nonthermally also by decay of heavy particles at far below the WIMP decoupling temperature. Any massive particle which interacts extra(-ordinarily) weakly is called E-WIMP. E-WIMPs might have never been in thermal equilibrium with photons. They are sketched in Fig. 2.11. Another particle whose number density does not follow Eq. (2.80) is the QCD axion. Also, baryon asymmetry that we discussed before does not follow Eq. (2.80). The asymmetric dark matter (ADM) idea follows the initial asymmetry generated by some conserved quantum number as in the baryogenesis based on quantum number B . We summarize them briefly in this subsection. More complete discussions of ADM will be presented in Chapter 8 after presenting theories of CDM from the particle theory perspective.

2.6.1. Nonthermal WIMP production

Inflaton can decay to produce heavy unstable particles after inflation. These decay products include thermal and nonthermal components [22]. WIMPs can be produced in this way also. In this subsection, the WIMP is denoted by X .

Let us begin the discussion in the standard inflationary scenario. The inflationary phase ends by the decay of the inflaton by reheating the Universe with relativistic particles, commonly denoted as “radiation”. The temperature attained by reheating is the reheating temperature T_{reh} . After reheating, the radiation-dominated Universe commences. Even the WIMP and other supermassive particles of our interest, generally at the multi-TeV mass range, are considered to be relativistic immediately after the reheating.

WIMP production by scattering

Suppose superheavy particles are produced by the inflaton decay. Immediately after the reheating is achieved, these superheavy particles are considered to be in thermal equilibrium. WIMPs are also in the thermal equilibrium. Consider the WIMP production by scattering of two superheavy particles,

$$X_1 + X_2 \rightarrow X + \dots \quad (2.86)$$

If the $X_1 + X_2$ scattering produces WIMPs above the WIMP decoupling temperature, the process is not affecting the thermal WIMP density (the green line in Fig. 2.11). If the process (2.86) produces WIMPs below the WIMP decoupling temperature, it is called nonthermal production of WIMPs. In Fig. 2.11, the nonthermally produced WIMP density is similar to the red curve marked as E-WIMP.

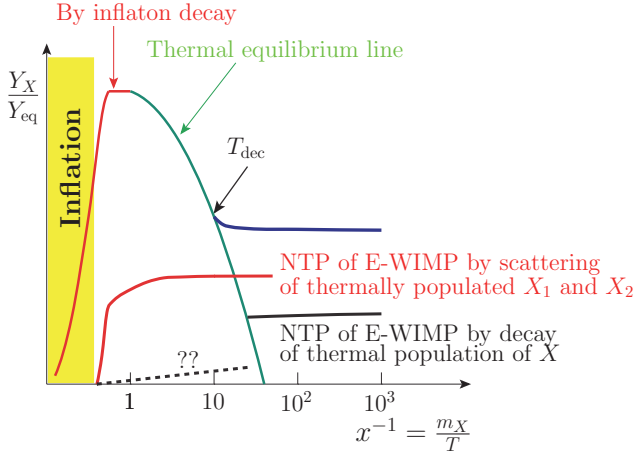


Fig. 2.11. Creation of E-WIMPs after inflation. The red curve shows schematically the NTP of E-WIMP by scattering of thermally populated X_1 and X_2 . The black curve shows schematically the NTP of E-WIMP by decay of thermally populated X when the cosmic time t reaches at $t_{\text{decay}} \approx 1/\Gamma$. The dashed black curve may be some contribution before X decays.

WIMP production by decay

With the subsequent evolution of the Universe, some of these particles (some after becoming nonrelativistic) decouple from the thermal plasma and the ratio of the number density of the decoupled particles to the entropy density is preserved. If the frozen-out particle is unstable, it finally decays to lighter particles which may include the DM:

$$\Phi \rightarrow X + \dots \quad (2.87)$$

By the decay of the mother particle Φ , the WIMP mass fraction is related to the original fraction Y_Φ by

$$Y_{\text{DM}}^{\text{NTP}}|_{T=T_{\text{D}}} = \frac{\alpha_X}{r_S} \text{Br}(\Phi \rightarrow \text{DM}) Y_\Phi|_{T=T_{\text{D}}}, \quad (2.88)$$

where α_X is the number of DM produced per one Φ , $r_S \equiv S_f/S_0$ is the ratio of the entropy before and after the Φ decay, and $\text{Br}(\Phi \rightarrow \text{DM})$ is the branching ratio of the DM productions from the decay of Φ . Here, T_{D} denotes the temperature of radiation at the time of Φ decay. Various possibilities are reviewed in Ref. [22].

2.6.2. E-WIMP production

E-WIMP interaction is characterized by much more weaker interaction than the weak interaction. The intrinsic interaction mass scale of an E-WIMP is larger than the W boson mass. Gravitational interaction has the Planck mass $M_{\text{P}} (\gg M_W)$, and the axion (a kind of Goldstone boson) has the decay constant $f_a (\gg M_W)$. Other kinds of E-WIMPs can have such suppressing masses around the interaction mediator scale.

As a typical example, consider an extra-weak interaction suppressed by f_a corresponding to the symmetry breaking scale of a global symmetry. For a heavy massive particle CDM, the corresponding Goldstone boson cannot be considered. The pseudo-Goldstone boson axion can be CDM and its superpartner *axino* can be an E-WIMP discussed here. In this case, the evolution equation of the axino number density is

$$\begin{aligned} \frac{dn_{\tilde{a}}}{dt} + 3Hn_{\tilde{a}} &= \sum_{i,j} \langle \sigma(i+j \rightarrow \tilde{a} + \dots) v_{\text{Moe}} \rangle n_i n_j \\ &+ \sum_i \langle \Gamma(i \rightarrow \tilde{a} + \dots) v_{\text{Moe}} \rangle n_i, \end{aligned} \quad (2.89)$$

where the first term on the RHS is the production by scattering and the second term is the production by decay. Both the scattering and the decay productions are suppressed by $1/f_a^2$. These features are presented in Fig. 2.11. For the NTP of WIMP, some M_W scale mass appears instead of f_a .

2.6.3. *ADM production*

Following the idea of baryon number generation out of $\Delta B = 0$ Universe, the idea of asymmetric dark matter (ADM) is suggested. The asymmetry generated is between DM particles and their antiparticles (anti-DM). Related to some quantum number, consider the dark matter number D . The asymmetry ΔD between DM and anti-DM remains constant after the annihilation of the symmetric components. In this case, the ADM relic density is set by ΔD in their initial populations, and not by the thermal freeze-out. Thus, it is a kind of NTP.

To generate ΔD , the mechanism should satisfy Sakharov's three physical conditions presented in Section 2.4. An interesting scenario is that the origins of the D asymmetry and of the B asymmetry can be related [52]. The asymmetry can be created in one of the D and B sectors at high temperatures and then subsequently transferred to the other sector such as by the sphaleron effect in the SM [44], or both asymmetries can be created together at the same moment. At low temperatures, the interactions for generating and transferring asymmetries are frozen. Another obvious mechanism is to relate the B asymmetry to the D asymmetry via a heavy particle which decays to both B and D sectors. Various mechanisms for DM production in the ADM models are reviewed in Refs. [53–55].

If $\Delta B = \Delta D$ is obtained,⁷ the ratio of ADM mass and the proton mass corresponds to their ratio in the cosmic energy pie, $28\%/5\% \simeq 5.5$. Then, m_D is predicted to be in the range 5–6 GeV. This region belongs to the light DM case, which the DAMA/LIBRA collaboration has suggested for a long time [56]. But, it has not been confirmed yet [57].

2.6.4. *Axion production*

If a scalar or pseudoscalar particle lived long enough to have survived and has a coherent motion now, the corresponding BCM can behave like CDM [4]. The CDM possibility in connection with the invisible axion coupling was originally proposed in 1983, which will be discussed in Chapter 6. A real scalar or pseudoscalar field ϕ has an effective potential of the form

$$V = \frac{m^2}{2}\phi^2 + (\cdots). \quad (2.90)$$

If mass m is sufficiently small, then some time in the late Universe $m = 3H$ will be satisfied. Let this time be t_{BCM} . Figure 2.12 shows a bullet representing the same value $\langle\phi\rangle$ in the region inside the horizon scale. Before t_{BCM} , $\langle\phi\rangle$ stays at the bullet. For $t > t_{\text{BCM}}$, $\langle\phi\rangle$ rolls down and oscillates around the minimum with the oscillation frequency m . Then, the energy density (kinetic energy plus potential energy) due

⁷ ΔD is defined in the same way as ΔB is defined in Eq. (2.69).

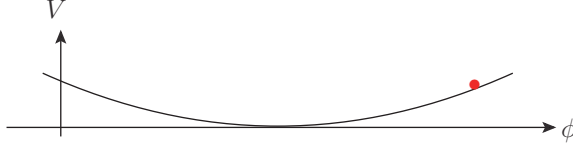


Fig. 2.12. A potential shape of ϕ . The bullet is at the time $m \simeq 3H$.

to this bullet oscillation averaged over one cycle is

$$\langle \rho \rangle = \frac{1}{2} \langle \dot{\phi} \rangle^2 + \frac{m^2}{2} \langle \phi \rangle^2,$$

and we have $\langle \dot{\phi} \rangle^2 = m^2 \langle \phi \rangle^2 = 2\langle V \rangle$. It is like harmonic oscillator motion in quantum mechanics.

We can consider the action

$$\int \sqrt{-g} \left(-\frac{1}{2} \partial_\mu \phi \partial^\mu \phi + \frac{1}{2} m^2 \phi^2 + \dots \right),$$

where $\dots$ is negligible compared to the m^2 term for a potential of the form shown in Fig. 2.12. Thus, the field ϕ satisfies the following equation in the evolving Universe,

$$\frac{d^2}{dt^2} \phi + 3H \frac{d}{dt} \phi + m^2 \phi \simeq 0. \quad (2.91)$$

Now, we have $\dot{\rho} = \dot{\phi}\ddot{\phi} + m^2\phi\dot{\phi} + \dot{m}m\phi^2$, and using Eq. (2.91), we obtain

$$\dot{\rho} = \dot{\phi}(-3H\dot{\phi} - m^2\phi) + m^2\phi\dot{\phi} + \dot{m}m\phi^2 = -3H\dot{\phi}^2 + \dot{m}m\phi^2, \quad (2.92)$$

which can be written as $\dot{\rho} + 3H\rho - \dot{m}m\phi^2 = 0$. Then, averaging over one cycle, it can be written as

$$\langle \dot{\rho} \rangle + 3\frac{\dot{R}}{R} \langle \rho \rangle - \frac{\dot{m}}{m} \langle \rho \rangle = 0, \quad (2.93)$$

which satisfies

$$\frac{d}{dt} \left(\frac{\langle \rho \rangle R^3}{m} \right) = 0 \quad (2.94)$$

Equation (2.94) shows that the BCM energy density $\langle \rho \rangle$ for constant m behaves like a conserved number in the comoving volume, which is the reason that BCM behaves as CDM.

At t_{BCM} , the oscillation rate of BCM is compared to the Hubble expansion rate, $1/3H$. If the oscillation rate is smaller than the Hubble expansion rate, $m > 3H$,⁸ it effectively stays at the bullet point. In this phase, there is only the potential energy V . On the other hand, if the oscillation rate is greater than the Hubble expansion

⁸We inserted the factor 3 from the cosmic evolution equation of $\langle \phi \rangle$.

rate, $m < 3H$, the bullet oscillation shown in Fig. 2.12 contains both potential and kinetic energies. In this BCM scenario, two conditions are satisfied to estimate its energy density:

- The mass parameter should remain (almost) constant.
- The commencing time of BCM is t_{BCM} when the cosmic temperature is denoted as T_{BCM} or T_1 [4].

In Section 6.1.1 of Chapter 6, we will discuss that Goldstone bosons must go into the bottleneck period, by going into the linearization process (to Eq. (2.93)) of the differential equation, which lowers T_{BCM} somewhat and lowers the allowed upper bound of the decay constant of the Goldstone boson. These have been studied recently [58].

2.6.5. Heavy lepton as WIMP

In this section, we present the simplest WIMP example — a heavy lepton where the interaction strength is precisely known. The charged current cross-section for

$$L(p) + \nu(k) \rightarrow N(p') + e(q), \quad (2.95)$$

is calculated. The T matrix element from the charged current interaction is

$$\begin{aligned} T &= \frac{G_F}{\sqrt{2}} \langle e(q), N(p') | \bar{e} \gamma^\mu (1 + \gamma_5) \nu_e \bar{N} \gamma_\mu (1 + \gamma_5) L | \nu(k), L(p) \rangle \\ &= \frac{G_F}{\sqrt{2}} \bar{u}_e(q) \gamma^\mu (1 + \gamma_5) u_\nu(k) \bar{u}_N(p') \gamma_\mu (1 + g_A \gamma_5) u_L(p), \end{aligned} \quad (2.96)$$

where the axial form factor g_A of heavy leptons is included explicitly, even though it is 1 because of the lack of strong interaction. The sign is $g_A > 0$ in our notation of γ_5 in the “ $V - A$ ” theory. Thus, we obtain

$$\sum_{\text{ini spin average, fin spin sum}} |T|^2 = \frac{G_F^2}{2} \frac{1}{2 \cdot 1} \sum_{\text{all spins}} (\cdots), \quad (2.97)$$

where we considered (incoming) two spin states of L and one spin state of ν and

$$\begin{aligned} (\cdots) &= [\bar{u}_e(q) \gamma^\mu (1 + \gamma_5) u_\nu(k) \bar{u}_\nu(k) \gamma^\alpha (1 + \gamma_5) u_e(q)] \\ &\quad \times [\bar{u}_N(p') \gamma_\mu (1 + g_A \gamma_5) u_L(p) \bar{u}_L(p) \gamma_\alpha (1 + g_A \gamma_5) u_N(p')]. \end{aligned}$$

Thus, we obtain

$$\begin{aligned} (2.97) &= \frac{G_F^2}{4} [\text{Tr } \gamma^\mu (1 + \gamma_5) \not{k} \gamma^\alpha (1 + \gamma_5) \not{q}] \\ &\quad \times [\text{Tr } \gamma_\mu (1 + g_A \gamma_5) (\not{p} + m) \gamma_\alpha (1 + g_A \gamma_5) (\not{p}' + m')] \end{aligned} \quad (2.98)$$

$$\begin{aligned}
&= \frac{G_F^2}{4} [\text{Tr } 2(1 - \gamma_5) \gamma^\mu \not{k} \gamma^\alpha \not{q}] \\
&\quad \times [\text{Tr } (1 + g_A^2 - 2g_A \gamma_5) (\gamma_\mu \not{p} \gamma_\alpha \not{p}' + m \gamma_\mu \gamma_\alpha \not{p}' + m' \gamma_\mu \not{p} \gamma_\alpha)] \\
&\quad + mm' \text{Tr } (1 - g_A^2) \gamma_\mu \gamma_\alpha],
\end{aligned} \tag{2.99}$$

which becomes

$$\begin{aligned}
(2.97) &= \frac{G_F^2}{4} 2[4(k^\mu q^\alpha + k^\alpha q^\mu - g^{\mu\alpha} k \cdot q) - 4i\epsilon^{\mu\nu\alpha\beta} k_\nu q_\beta] \\
&\quad \times [4(1 + g_A^2)(p_\mu p'_\alpha + p_\alpha p'_\mu - g_{\mu\alpha} p \cdot p') + 4mm'(1 - g_A^2)g_{\mu\alpha} \\
&\quad - 8g_A(i)\epsilon_{\mu\rho\alpha\sigma} p^\rho p'^\sigma] \\
&= \frac{G_F^2}{4} \cdot 2 \cdot 4[(1 + g_A)^2(2k \cdot pq \cdot p' + 2k \cdot p'q \cdot p) - (1 - g_A^2)mm'k \cdot q] \\
&= 4G_F^2 \left[(1 + g_A)^2(k \cdot pq \cdot p' + k \cdot p'q \cdot p) - \frac{1}{2}(1 - g_A^2)mm'k \cdot q \right].
\end{aligned} \tag{2.100}$$

As discussed in Section 4.6.1 of Chapter 4, we average over the $\pm \gamma_5$ conventions and we obtain

$$\begin{aligned}
(2.97) &\rightarrow \frac{1}{2} [(2.100)_{+\gamma_5} + (2.100)_{-\gamma_5}] \\
&= 2G_F^2 [(2 + 2g_A^2)(k \cdot pq \cdot p' + k \cdot p'q \cdot p) - (1 - g_A^2)mm'k \cdot q].
\end{aligned} \tag{2.101}$$

In the center-of-mass frame,

$$p = (E_L, \mathbf{p}), \quad k = (E, -\mathbf{p}), \quad p' = (E_N, -\mathbf{q}), \quad q = (E', \mathbf{q}), \tag{2.102}$$

we obtain $k \cdot p = EE_L + |\mathbf{p}|^2$, $q \cdot p' = E'E_N + |\mathbf{q}|^2$, $k \cdot p' = EE_N - \mathbf{p} \cdot \mathbf{q}$, and $q \cdot p = E'E_L - \mathbf{p} \cdot \mathbf{q}$. In this CM frame,

$$\begin{aligned}
(2.101) &= 2G_F^2(2 + 2g_A^2)(2E_LE_N EE' + E_NE'E\mathbf{p}^2 + E_LE\mathbf{q}^2 \\
&\quad + \mathbf{p}^2\mathbf{q}^2 + (\mathbf{p} \cdot \mathbf{q})^2 - [(E_NE + E_LE')\mathbf{p} \cdot \mathbf{q}]) \\
&\quad - 2G_F^2(1 - g_A^2)mm'(EE' + \mathbf{p} \cdot \mathbf{q})
\end{aligned} \tag{2.103}$$

from which we will neglect the terms containing $\mathbf{p} \cdot \mathbf{q}$ because they will disappear over the phase space integration. In the limit of relativistic leptons and nonrelativistic heavy leptons, $q \equiv |\mathbf{q}| \simeq E'$ and $\mathbf{p}/M_{L,N} \equiv p/M_{L,N} \simeq 0$.

$$(2.101) = 4G_F^2(1 + g_A)^2(2E_LE_N EE' + E_NE'E p^2 + E_LE q^2 + p^2 q^2(1 + \cos^2 \theta)).$$

It is integrated over the available phase space,

$$\begin{aligned}
& \frac{(2\pi)^{-2} 2G_F^2}{||\frac{\mathbf{p}}{E_L}|-1|} \int \frac{d^3\mathbf{p}' d^3\mathbf{q}}{2E_L 2E 2E_N 2E'} \delta^{(4)}(p+k-p'-q) \\
& \quad \times [(2+2g_A^2)(2E_L E_N EE' + E_N E' p^2 + E_L E q^2 + p^2 q^2 (1+\cos^2 \theta)) \\
& \quad + (g_A^2 - 1)mm' EE'] \\
& = \frac{G_F^2 (1+g_A)^2}{16\pi} \int \frac{dq q^2}{E_L E_N EE'} \int_{-1}^1 d\cos\theta \delta(E' + E_N - E_L - E) \\
& \quad \times [(2+2g_A^2)(2E_L E_N EE' + E_N E' p^2 + E_L E q^2 + p^2 q^2 (1+\cos^2 \theta)) \\
& \quad + (g_A^2 - 1)mm' EE'] \\
& = \frac{G_F^2 (1+g_A)^2}{8\pi} \int \frac{dq q^2}{E_L E_N EE'} \delta\left(q + m_N + \frac{q^2}{2m_N} - m_L - \frac{k^2}{2m_L} - k\right) \\
& \quad \times \left(2m_L m_N kq + \frac{m_N k^3 q}{m_L} + \frac{m_L q^3 k}{m_N} + \frac{k^3 q^3}{2m_L m_N} + E_N k^2 q + E_L k q^2 \right. \\
& \quad \left. + \frac{4}{3} k^2 q^2\right) + \frac{G_F^2 (g_A^2 - 1)mm'}{16\pi} \int \frac{dq q^2}{E_L E_N EE'} \delta\left(q + m_N + \frac{q^2}{2m_N} \right. \\
& \quad \left. - m_L - \frac{k^2}{2m_L} - k\right) EE',
\end{aligned}$$

where the scalar integration variables are $p = |\mathbf{p}|$ and $q = |\mathbf{q}|$. For the incoming momentum $\mathbf{p}$, the value q is fixed as

$$\sqrt{m_L^2 + k^2} - \sqrt{m_N^2 + q^2} = +q - k, \quad (2.104)$$

where

$$\begin{aligned}
q & = \frac{k(m_L^2 + m_N^2)}{2m_L^2} \left(1 - \left[1 + \frac{m_L^2(m_L^2 - m_N^2)^2}{k^2(m_L^2 + m_N^2)^2} - \frac{4m_N^2 m_L^2}{(m_L^2 + m_N^2)^2}\right]^{1/2}\right) \\
& \simeq k \left(\frac{m_N^2}{(m_L^2 + m_N^2)} - \frac{(m_L^2 - m_N^2)^2}{4k^2(m_L^2 + m_N^2)}\right)
\end{aligned} \quad (2.105)$$

with $k^2 \geq (m_L^2 - m_N^2)^2/m_N^2$. In the nonrelativistic region of heavy leptons, the above integration gives $G_F^2(2+2g_A^2)q^2/2\pi + G_F^2(g_A^2-1)q^2/2\pi = G_F^2(1+3g_A^2)q^2/2\pi$.

If N is not a composite particle, the above calculation is valid for $g_A = 1$ which is equivalent to $(1+3g_A^2) = (1+g_A)^2$. But if N is composite, then g_A need not be 1. Presumably, the confining interaction preserves the parity symmetry as in QCD. Then, we have to average over the γ_5 conventions as discussed in Section 4.6.1 of Chapter 4. The same argument applies to the neutron decay and nucleon-lepton scattering discussed in Section 2.3.

Exercise

1. Consider the process $\nu_\mu + \bar{\nu}_\mu \rightarrow \nu_\tau + \bar{\nu}_\tau$ with the following interaction:

$$\mathcal{H}_{\text{NC}} = -\frac{G_F \cos^2 \theta_W}{2\sqrt{2}} \bar{\nu}_\mu \gamma^\alpha (1 + \gamma_5) \nu_\mu \bar{\nu}_\tau \gamma_\alpha (1 + \gamma_5) \nu_\tau. \quad (2.106)$$

In the relativistic energy regime, i.e., $E_{\nu_i} \gg m_{\nu_i}$, obtain the scattering cross-section given in Eq. (2.39) for $\nu_\mu(E, \mathbf{p}) + \bar{\nu}_\mu(E, -\mathbf{p}) \rightarrow \nu_\tau(E, \mathbf{p}') + \bar{\nu}_\tau(E, -\mathbf{p}')$,

$$|T|^2 = 2G_F^2 E^4 (1 + g_{A,\text{lep}}^2) \cos^2 \theta_W [4 + (1 - \cos \theta)^2]. \quad (2.107)$$

2. Obtain the scattering cross-section for $p + e^- \rightarrow n + \nu_e$ with the kinetic energies of the order of 1 MeV. Use the following “ $V - A$ ” interaction,

$$\mathcal{H}_{\text{int}} = -\frac{G_F \cos \theta_C}{\sqrt{2}} \bar{n} \gamma^\alpha (1 + \gamma_5) p \bar{\nu}_e \gamma_\alpha (1 + \gamma_5) e. \quad (2.108)$$

3. Show that the denominator and the numerator of Eq. (2.85) for $m_a = m_b = m$ become

$$D = \left[4\pi m^2 T K_2 \left(\frac{m}{T} \right) \right]^2, \quad (2.109)$$

$$N = \int_{4m^2}^{\infty} \sigma(s - m^2) \sqrt{s} K_1 \left(\frac{\sqrt{s}}{T} \right) ds, \quad (2.110)$$

where $K_{1,2}$ are the modified Bessel functions and s is the total energy squared in the CM frame, $s = (p_a + p_b)^2$.

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Chapter 3

Dark Matter and Large-Scale Structures in the Universe

I insist upon the view that “all is waves” — E. Schrödinger

Studying motion of galaxies in the Coma cluster, Zwicky suggested the existence of nonluminous mass at the cluster scale [1]. Nowadays, the nonluminous matter is called dark matter in the particle physics jargon. Dark matter (DM), being composed of very weakly interacting elementary (or composite) particles, must be present in all astrophysical scales, from the Universe of the horizon size down to solar and even down to Earth scales. In particle physics, DM candidates are broadly classified to the bosonic coherent motion (BCM) and weakly interacting massive particles (WIMPs), which will be theoretically presented in Chapters 4, 6 and 7. The detection strategy of DM at laboratories will be discussed in Chapter 9.

At present, the evidences for the existence of DM are only of astrophysical origin. So, in this chapter, we glimpse (i) what are these astrophysical evidences, (ii) density perturbation which arises from quantum fluctuation and is the basic ingredient for forming galaxies, and (iii) summarize some results of the N -body simulations in the Λ CDM model.

3.1. Astrophysical hints of CDM

3.1.1. Flat rotation velocities

The first cosmological evidence on DM was found from the flattening of the rotation velocity curve of stars at far distances from the galactic center [2].

The rotating spiral galaxies have stars rotating in the arms. If most mass of a galactic mass M_{gal} is at the center, Newton’s gravitational force at r would give the transverse acceleration $v^2/r = F/m_{\text{inside}} \propto 1/r^2$, i.e., the rotation velocity behaves like $\propto 1/\sqrt{r}$. Note also that galaxies have more gas and dust than the

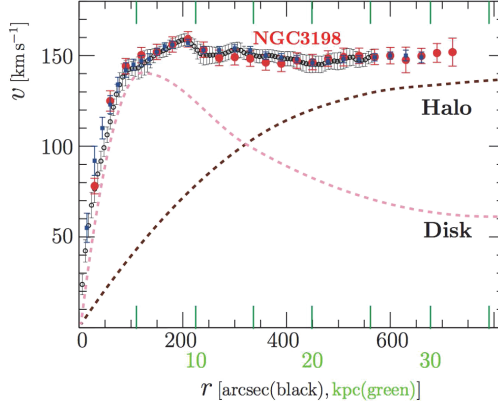


Fig. 3.1. Data of NGC 3198 on the rotation velocity (v) vs. distance (r) plane. Full red points are from [3], open black points are from [4] based on the THINGS data, and blue squares are from [5] based on the WRST data.

visible stars in them. Figure 3.1 shows the effects of gas contribution in NGC 3198 to the rotation velocities, which is compiled in Ref. [3]. Here, data from the H_I Nearby Galaxy Survey (THINGS) [4] and the Westerbork Synthesis Radio Telescope (WRST) [5] are used. The red bullets were studied in [3]. Dashed lines are the expected velocities for the halo and disc contributions. The disc velocity is a bit above $1/\sqrt{r}$ at large r . The data points can be fitted [3] by adding the halo and disc curves by $a(\text{halo}) + b(\text{disc})$. This hints that there must be nonluminous matter at large distances in the galactic halo.

3.1.2. Observation of galaxies by gravitational lensing

In general relativity, light follows geodesics, hence it is bent when it passes around the curved spacetime. Thus, a massive object can act as a lens for lights passing through it to an observer sitting on the other side of the massive object. A gravitational lens can be considered as a distribution of matter (such as a cluster of galaxies) between a distant light source and an observer. Thus, gravitational lens effect is the direct method of measuring dark mass.

Figure 3.2 shows the lights passing the most massive galaxy clusters Abell 1689 by NASA's Hubble Space Telescope. Interspersed with the foreground cluster are thousands of galaxies. Some of gravitationally lensed images are marked here [7]. This gravitational lens is another evidence that there exists DM at the galactic cluster scale.

3.1.3. Clusters of galaxies

In fact, the first suggestion of DM in the Universe was made from the Coma cluster for which motion of galaxies was not accountable only by the luminous mass in

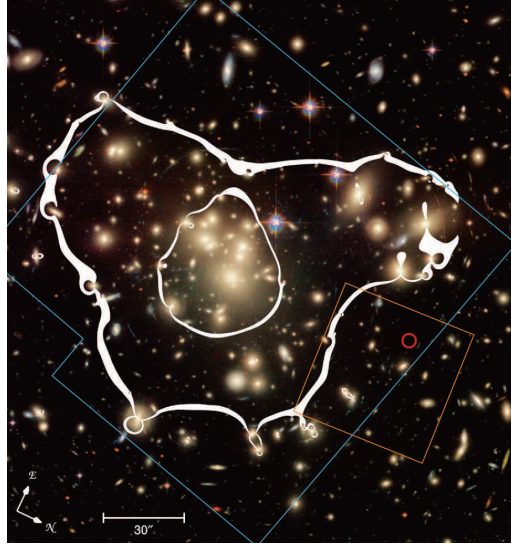
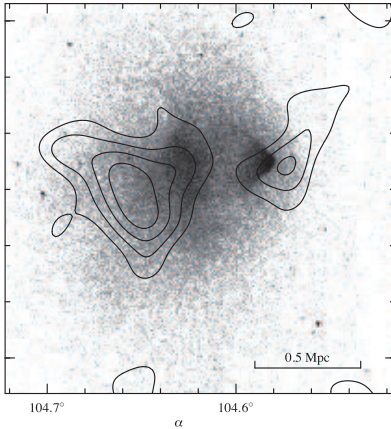


Fig. 3.2. NASA's Hubble Space Telescope image of the most massive galaxy clusters Abell 1689 [7].



Markevitch *et al.* (2004)

(a)



A gas image of Bullet cluster

(b)

Fig. 3.3. (a) Profiles of the bullet Cluster [6], and (b) color coding of (a). In (b), one can visualize the colliding clusters with the blue-colored DM gas moving ahead.

the cluster. So, Zwicky suggested the existence of nonluminous mass in the Coma cluster [1] which we now call DM. A galaxy cluster consists of hundreds to thousands of galaxies with typical masses ranging from $10^{14-15} M_{\odot}$.

The most visual piece of evidence for DM is shown from photos of colliding galaxy clusters. The Bullet Cluster shown in Fig. 3.3 is such an example. Two

galaxy clusters are brought together by their mutual gravitational attraction. When clusters collide, the compact objects like stars pass through, but the diffuse gas of one cluster can meet the diffuse gas of another cluster. If the interaction strength is large, they can collide and the collided gas is slowed down. The atoms composed of the SM particles are slowed down by these collisions. But DM particle interactions with atoms and their self-interactions are sufficiently small such that the movements of DM particles are not hindered in this way. When atoms collide, the gas is heated up and emits X-rays which can be observed by X-ray telescopes. The existence of passing-by DM particles can be inferred by the gravitational lensing. For the Bullet Cluster profile [6] in Fig. 3.3 (a), color coding of the X-ray observation is shown in pink and DM, by the effect of gravitational lensing, is shown in blue in Fig. 3.3 (b). This picture shows the un-hindered DM particles moving ahead of the dragged atoms.

3.1.4. Cosmic evolution

Also, a hint that the existence of DM is essential comes from the early history of the Universe in the inflation models. As such, this kind of model-dependent study may not be a direct evidence on DM. Nevertheless, it can be at least a hint since only the inflation idea successfully calculates the cosmic observables without any severe contradictions. Interpretation of the WMAP and Planck data on cosmic microwave background radiation (CMBR) in the Λ CDM model determines the percentages of the energy pie of Fig. 1.2. This is drawn by varying the cosmic evolution parameters in the Λ CDM model and comparing their calculation to the observed baryons.

In Fig. 3.4, the WMAP data is compared to the observed baryons. In (a), the WMAP data for five years is shown as dark gray stripe. The dashed-dotted line is the fit to the measured points, and the dashed line is the fit to the points of (b) with some corrections performed in [8]. Roughly, 5% is not counted by gas, stars, and corrections. So, 83% of mass is in DM.

The Planck Collaboration varied six parameters in the Λ CDM model, $\Omega_{\text{baryon}} h^2$, $\Omega_{\text{CDM}} h^2$, $100 \theta_{\text{MC}}$, τ , n_s , and $\log(10^{10} A_s)$, and calculated¹

$$\Omega_{\Lambda}, \Omega_{\text{baryon}}, \sigma_8, z_{\text{re}}, h, n_s, \tau_{\text{U}}, \log(10^9 A_s), \text{ etc.}, \quad (3.1)$$

which are within the measured values [9]. Among these, parameters related to manufacturing the inhomogeneities in the Universe are related to DM (or CDM). Figure 3.5 shows the temperature correlations observed by the Planck collaboration [9]. Here, ℓ shows the harmonics, and C_{ℓ} in the vertical axis is calculated in the inflating Universe in the flat Λ CDM model. C_{ℓ} depends on six main parameters

¹See page xii for these names.

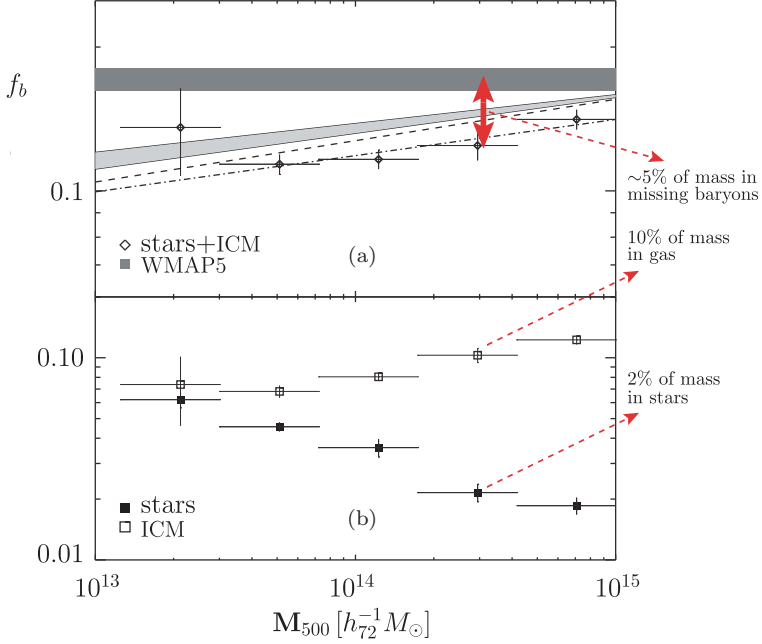


Fig. 3.4. The baryon fraction f_b among DM [8]. The total baryonic fraction is obtained from the ratio of the average gas and stellar masses.

of Eq. (3.1),

$$C_\ell = \sum_k G(\ell, k) P(k), \quad (3.2)$$

$$P(k) = A_s \left(\frac{k}{k_*} \right)^{n_s - 1}, \quad (3.3)$$

where $G(\ell, k)$ is a function of Ω_{baryon} , Ω_{DM} , h and τ . The expressions for P_s [11, 12] and $n_s - 1$ in the inflaton model [13] are given by

$$\frac{4\pi k^3}{(2\pi)^3} P_s(k) = A_s \left[\frac{H^2}{2\pi\dot{\phi}} \right]_{k/a=H}^2 = A k^{n_s - 1}, \quad (3.4)$$

$$n_s - 1 = M_{\text{P}}^2 \left(2 \frac{V''}{V} - 3 \left[\frac{V'}{V} \right]^2 \right). \quad (3.5)$$

The peak around $\ell = 220$, marked as a green dashed line, is the scale determined by the cold dark matter (CDM) acoustic waves. The function $\sin \ell \theta$ has the angular spacing π/ℓ for the half wavelength for the mode. Thus, $\ell \simeq 220$ corresponds to $\approx 1.5^\circ$ angular spacing.

Figure 3.6 shows the cosmic map of temperature profile right after the recombination time, about 380,000 years after the Big Bang. Here, high CDM density

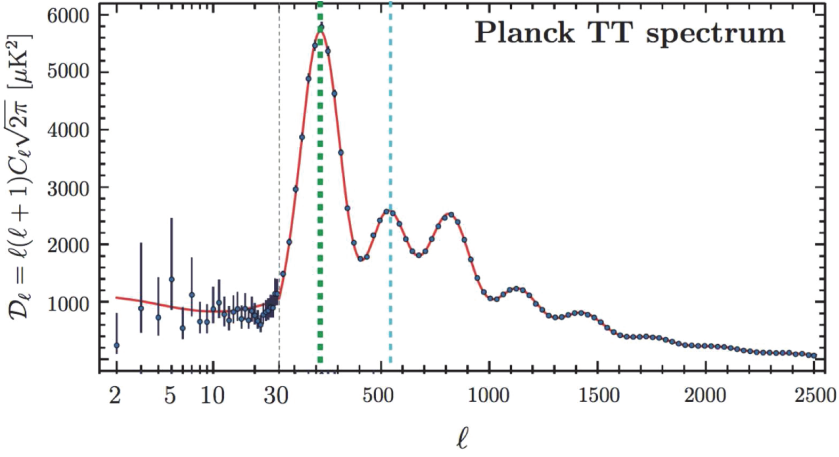


Fig. 3.5. The Planck TT spectrum as a function of multipole ℓ [10].

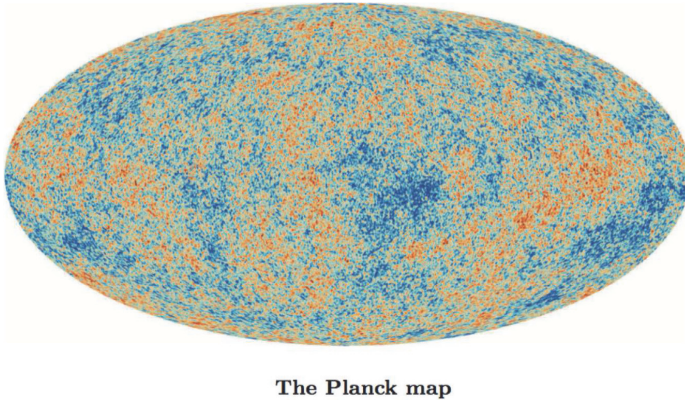


Fig. 3.6. The Planck CMBR data.

regions are close to the blue color and the low density regions are close to the red color. Thus, the angular spacing between the blue points is expected to be $\sim 1^\circ$. This size is interpreted as a typical galactic scale. The next peaks represent larger size acoustic waves. The first peak is the dominant one and the second is the peak due to under-density, the third peak is due to over-density, etc. Thus, the peaks around $\ell \simeq 530$, marked as a skyblue dashed line, and the third peak may correspond to the next important perturbation, i.e., the perturbation of baryon asymmetry. But, note that this is the present observation expanded from the one around the recombination time. From the Sachs–Wolfe effect, the actual photon temperature distribution at recombination is the opposite from present observational CDM density anisotropy. The red is higher temperature and the blue is lower temperature. A simple explanation is the following. Consider a photon from cosmic time 380,000 yrs,

when densities of both photon and CDM are high. When the photon leaves the place where the gravitational potential is high due to the large density, it is red-shifted more at higher density region. This means the red-shifted photons that we observed now were bluer if they came from higher density region.

It is known that the Einstein–Podolsky–Rosen (EPR) paradox [14] is not a paradox but a correlation given in quantum mechanics. A hidden variable theory by assuming locality, a possibility in classical mechanics, gives Bell’s inequality [15]. Bell’s inequality has been shown to be violated by 5σ [16] and quantum mechanical wave description is not forbidden by EPR. Thus, the amplitude given by quantum wave during the inflationary phase is a physical description correlating one part of the wave function with another part of the wave function. When this wave function enters into the horizon, one part of the gravitational potential (or wave function) has a correlation with the other parts. This is the way the homogeneity is understood in inflation.

3.1.5. Nucleosynthesis

The amount of atoms in the Universe is a known quantity. There are two ways to obtain the amount of DM in the Universe. One is to calculate locally using the vertical kinematics of stars near Sun — called tracers [17]. Let us denote it as ρ_{dm} . The other is a global one. The velocities of stars in far away regions from the galactic center satisfy the flat rotation curve relation. Extend it to Sun’s position, and determine the density. Let us denote it as $\rho_{\text{dm,extr}}$. A naive guess is that they are the same. In Fig. 3.7 (a), the gray band is ρ_{dm} . As time goes on, the error bars decrease. From this figure, the DM density at the solar system is $(0.2\text{--}0.6) \cdot \text{GeV cm}^{-3}$, and usually $(0.3\text{--}0.45) \text{ GeV cm}^{-3}$ is assumed in the DM detection experiments. The determination of DM near Sun is based on the known density of baryons near Sun.

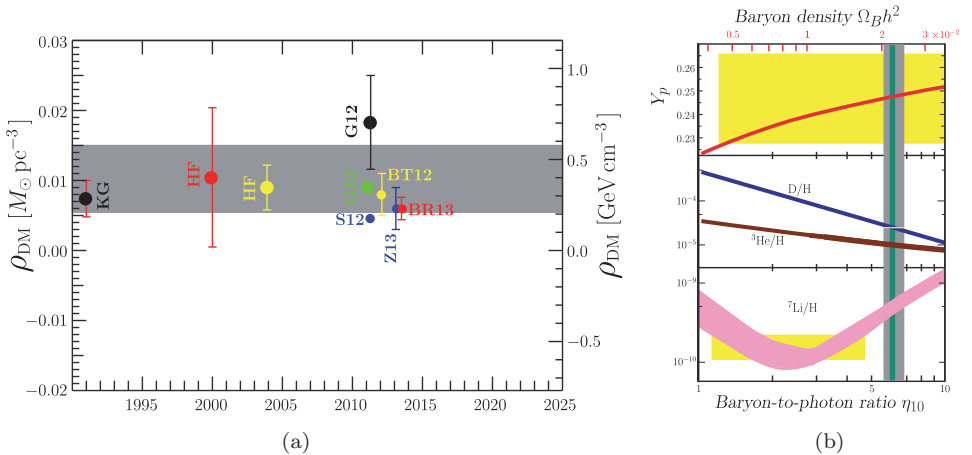


Fig. 3.7. (a) The local DM density discussed in Chapter 9, and (b) the primordial abundances of light elements from nucleosynthesis as functions of the baryon/photon ratio.

The baryon density at the time of its creation by baryogenesis, discussed in Chapter 8, cannot be measured now. The earliest time restricting giving the current bound is the era of nucleosynthesis. The primordial abundances of light element depend on the baryon density at that era. The baryon density during nucleosynthesis is shown in Fig. 3.7 (b) which is consistent with 5 % in the energy pie. The current nonluminous baryons, baryons in Jupiter size objects or those swallowed by black holes, must be included in this number at the time of nucleosynthesis. The baryon to photon ratio at present is

$$\frac{\rho_b}{\rho_\gamma} \simeq 0.6 \times 10^{-9} \quad (3.6)$$

which is marked as the green line in Fig. 3.7 (b).

3.2. Density perturbation

3.2.1. Quanta

It is most astonishing that quantum fluctuations have influenced the evolution of the Universe so profoundly. The observed inhomogeneity shown in Fig. 3.6 right after the recombination time is a consequence of quantum fluctuations. This possibility was suggested in Ref. [18], which was later used in inflationary models [19]. Sometime after recombination, galaxies formed at the scale ℓ_{Gal} , as shown in Fig. 3.6. Max Born was the first to discover (by chance and with no theoretical foundation) that the square of the quantum wave function could be used to predict the probability where the particle would be found [20]. In cosmological evolution, the relevant wave function is contained in the metric $g_{\mu\nu}$.

The density perturbation $\delta\rho$ can be measured by the temperature autocorrelation as in Fig. 3.6. With the assumption $\delta\rho \propto \delta T$, $\langle(\bar{\rho}(\mathbf{r}) + \delta\rho(\mathbf{r}))(\bar{\rho}(\mathbf{r}') + \delta\rho(\mathbf{r}'))\rangle - \langle(\bar{\rho}(\mathbf{r}))(\bar{\rho}(\mathbf{r}'))\rangle \propto \langle T(\mathbf{r})\delta T(\mathbf{r}')\rangle$. Figure 3.5 shows the temperature autocorrelation, $\sqrt{C_{220}} \sim 1.3 \times 10^{-4}$ K, at the first peak. Since $RT = (\text{constant})$, the redshift at this recombination time was about $z \sim 1000$.

For the acoustic oscillation, let us use the sphere normalization with the spherical Bessel function of the first kind,

$$j_\nu(\xi) = \sqrt{\frac{\pi}{2\xi}} J_{\nu+\frac{1}{2}}(\xi), \quad (3.7)$$

where $J_{\nu+\frac{1}{2}}(r)$ is the half-integer-order Bessel function. The first few spherical Bessel functions are

$$j_0(\xi) = \frac{\sin \xi}{\xi}, \quad (3.8)$$

$$j_1(\xi) = \frac{\sin \xi}{\xi^3} - \frac{1}{\xi} \cos \xi, \quad (3.9)$$

$$j_2(\xi) = \left(\frac{3}{\xi^2} - \frac{1}{\xi} \right) \sin \xi - \frac{3 \cos \xi}{\xi^2}, \text{ etc.} \quad (3.10)$$

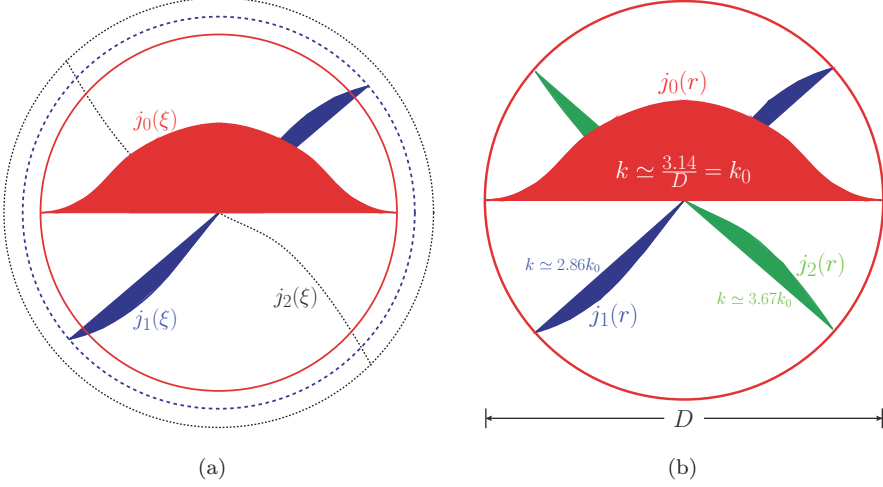


Fig. 3.8. Profiles of spherical Bessel functions j_0 , j_1 , and j_2 . (a) The first zeros at $\xi \neq 0$ are shown as spheres of solid red, dashed blue, and dashed black arcs, and (b) wave numbers in a sphere of diameter D with the sphere normalization, $j_n(\frac{D}{2}) = 0$.

Figure 3.8 shows the above spherical Bessel functions. The first zeros of $j_0(\xi)$, $j_1(\xi)$, and $j_2(\xi)$ for $\xi > 0$ at Fig. 3.8(a) are $\xi_0 = \pi$, $\xi_1 \simeq 4.493$, and $\xi_2 \simeq 5.763$, respectively. With the sphere normalization, Fig. 3.8(b) shows the wave numbers for the first modes of $j_{0,1,2}(r)$.

The acoustic waves are stationary waves with the nodes at the horizon. For example, imagine an oscillating red profile of Fig. 3.8(b) for the lowest mode. These acoustic waves oscillate as

$$\sim e^{i\omega t} \quad (3.11)$$

even after the horizon scale engulfs many wavelengths. Within this horizon scale, the acoustic waves are stationary waves. But, before the horizon crosses the scale ℓ_{Gal} , the expansion is inflationary, i.e., $D \propto e^{H_{\text{infl}} t}$ and the mode was NOT in an oscillatory form. The shape of the wave profile is fixed and simply exponentially expanding. This exponential expansion is the key relating the microscopic scale λ to the cosmic scale $a\lambda$ where a is the scale factor. An illustrative (nonrigorous) equation for the mode is

$$u_k'' + \left(k^2 - \frac{a''}{a} \right) u_k = 0, \quad (3.12)$$

where prime denotes the derivative with respect to the conformal time and a is the scale factor. In the inflationary phase where $a''/a = H_{\text{infl}}^2$ is constant and large, the mode expands exponentially. But after the exit from the inflation, $a''/a \propto t^{-3/2}$ which is negligible compared to k^2 , we obtain an acoustic oscillatory mode. This stationary mode is in the metric and behaves as a gravitational potential

well. Thus, the energy inhomogeneities flow into this potential well. These energy inhomogeneities are provided by CDM just before the recombination time. This is the reason why CDM is the seed of galaxy formation. To relate this density inhomogeneity to the temperature inhomogeneity, we assumed the following:

- The temperature inhomogeneity arises from the baryon inhomogeneity.
- The baryon inhomogeneity follows the CDM inhomogeneity.
- The CDM inhomogeneity is the result of CDM particles placed in the gravitational potential well.

The current wisdom is that the quanta u_i of Fig. 3.8 are related to the metric perturbation. The Einstein equation determines the energy–momentum tensor perturbation.

3.2.2. Exit from inflation and horizon crossing

In a flat Robertson–Walker background, the metric can be written as [21, 22]

$$\begin{aligned} ds^2 = & -a^2(1+2\phi)d\eta^2 - 2a^2\left(B_{,i} + B_i^{(v)}\right)d\eta dx^i \\ & + a^2\left[(1+2\psi)\delta_{ij} - 2E_{,ij} \right. \\ & \left. + C_{i,j}^{(v)} + C_{j,i}^{(v)} + 2C_{ij}^{(t)}\right]dx^i dx^j, \end{aligned} \quad (3.13)$$

where $a(\eta)$ is the cosmic-scale factor, and we assume $B^{(v)i}{}_{,i} \equiv 0 \equiv C^{(v)i}{}_{,i}$ (transverse), and $C^{(t)j}{}_{i,j} = 0 = C^{(t)j}{}_{,j}$ (transverse-trace-free) with indices of $B_i^{(v)}$, $C_i^{(v)}$, and $C_{ij}^{(t)}$ raised and lowered by δ_{ij} as the metric; indices (v) and (t) indicate the vector- and tensor-type perturbations, respectively. Indices $i, j, \dots$ indicate spatial ones. Considering the linear perturbation theory, Mukhanov [23] suggested to take the longitudinal gauge conditions, $B = 0 = E$. Then, for the scalar-type perturbation, Eq. (3.13) becomes

$$ds^2 = -a^2(1+2\phi)d\eta^2 + a^2(1+2\psi)\delta_{ij}dx^i dx^j. \quad (3.14)$$

This metric is evolving under the influence of the energy–momentum tensor T_{ij} .

Since the Einstein tensor for the background metric ${}^{(0)}G_\nu^\mu$ is assumed to be diagonal, viz. Exercise 1, the energy–momentum tensor ${}^{(0)}T_\nu^\mu$ is diagonal,

$${}^{(0)}T_0^0 = -\frac{3M_{\text{P}}^2}{a^2}H^2, \quad {}^{(0)}T_i^0 = 0, \quad {}^{(0)}T_j^i = -\frac{M_{\text{P}}^2}{a^2}(2H' + H^2)\delta_j^i, \quad (3.15)$$

where $H = \dot{a}/a$. For the perturbation expansions of metric and the energy–momentum tensor, $G_\nu^\mu = {}^{(0)}G_\nu^\mu + \delta G_\nu^\mu + \dots$ and $T_\nu^\mu = {}^{(0)}T_\nu^\mu + \delta T_\nu^\mu + \dots$, one

can determine

$$M_{\text{P}}^2 \delta G_{\nu}^{\mu} \simeq \delta T_{\nu}^{\mu}. \quad (3.16)$$

As in Exercise 2, gauge invariant first-order Einstein tensors are constructed

$$\overline{\delta G}_0^0 = \delta G_0^0 - \left({}^{(0)}\delta G_0^0 \right)' (B - E'), \text{ etc.} \quad (3.17)$$

Thus, the gauge invariant equations for the perturbation are obtained,

$$\overline{\delta G}_{\nu}^{\mu} M_{\text{P}}^2 = \overline{\delta T}_{\nu}^{\mu}. \quad (3.18)$$

The left-hand side of the above equation is determined by the metric, i.e., in terms of ϕ and ψ . In the gauge chosen in Eq. (3.14), $\overline{\phi} = \phi$ and $\overline{\psi} = \psi$. The simplest gauge-invariant linear perturbations in the gauge Eq. (3.14) are Φ and Ψ [23],

$$\Phi \equiv \phi - \frac{1}{a}[a(B - E')] = \phi, \quad \Psi \equiv \psi + \frac{a'}{a}(B - E') = \psi. \quad (3.19)$$

Two relevant Einstein equations for Φ and Ψ are

$$M_{\text{P}}^2 [\Delta \Psi - 3H(\Psi' + H\Phi)] = \frac{1}{2}a^2 \overline{\delta T}_0^0, \quad (3.20)$$

$$M_{\text{P}}^2 \left\{ \left[\Psi'' + H(2\Psi + \Phi)' + (2H' + H^2)\Phi + \frac{1}{2}\Delta(\Phi - \Psi) \right] \delta_j^i - \frac{1}{2}(\Phi - \Psi)_j^i \right\} = -\frac{1}{2}a^2 \overline{\delta T}_j^i \quad (3.21)$$

where $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$. For a diagonal $\overline{\delta T}_j^i$, Φ and Ψ in Eq. (3.21) imply the condition, $\Phi = \Psi$. The energy-momentum tensor is written, assuming the perfect fluid

$$T_{\nu}^{\mu} = (\epsilon + p)u^{\mu}u_{\nu} + p\delta_{\nu}^{\mu}, \text{ i.e.,} \quad (3.22)$$

$$\overline{\delta T}_0^0 = -\overline{\delta \epsilon}, \quad \overline{\delta T}_j^i = -\overline{\delta p}\delta_j^i, \quad (3.23)$$

for which we obtain

$$M_{\text{P}}^2 [\Delta \Phi - 3H(\Phi' + H\Phi)] = \frac{1}{2}a^2 \overline{\delta \epsilon}, \quad (3.24)$$

$$M_{\text{P}}^2 [\Phi'' + 3H\Phi' + (2H' + H^2)\Phi] = -\frac{1}{2}a^2 \overline{\delta p}. \quad (3.25)$$

Isentropic perturbation

The right-hand side of Eqs. (3.24) and (3.25) contains functions of $\overline{\delta p}$ and $\overline{\delta \epsilon}$, which can be related in terms of another parameter $p(\epsilon, S)$ where S is entropy. The fluctuation $\overline{\delta p}$ can be expressed as

$$\overline{\delta p} = \left(\frac{\partial p}{\partial \epsilon} \right)_S \overline{\delta \epsilon} + \left(\frac{\partial p}{\partial S} \right)_\epsilon \delta S \equiv c_s^2 \overline{\delta \epsilon} + \tau \delta S, \quad (3.26)$$

where $|c_s|$ is the sound velocity.

$$\Phi'' + 3(1 + c_s^2)H\Phi' - c_s^2\Delta\Phi + [2H' + (1 + c_s^2)H^2]\Phi = -\frac{1}{2}a^2\tau\delta S. \quad (3.27)$$

3.2.3. Adiabatic perturbation

For $p = 0$ ($c_s = 0$) in the matter-dominated Universe $H = \frac{2}{\eta}$, we have

$$a \propto \eta^2, \quad H = \frac{2}{\eta}, \quad H' = -\frac{2}{\eta^2}, \quad (3.28)$$

and Eq. (3.27) becomes

$$\Phi'' + \frac{6}{\eta}\Phi' = 0, \quad (3.29)$$

which has a solution

$$\Phi = f_0(\mathbf{x}) + \frac{f_d(\mathbf{x})}{M_{\text{P}}^5 \eta^5}. \quad (3.30)$$

Thus, Eq. (3.24) becomes with $\epsilon_0 = \frac{12M_{\text{P}}^2}{a^2\eta^2}$,

$$\frac{\overline{\delta \epsilon}}{\epsilon_0} = \frac{1}{6} \left[\Delta f_0(\mathbf{x})\eta^2 - 12f_0(\mathbf{x}) + \frac{\Delta}{M_{\text{P}}^5 \eta^3} f_d(\mathbf{x}) + \frac{18}{M_{\text{P}}^5 \eta^5} f_d(\mathbf{x}) \right]. \quad (3.31)$$

If the physical scale $\lambda_{\text{ph}} \sim 2\pi a/k$ is much larger than the Hubble scale, i.e., $k\eta \ll 1$, we have, if we neglect f_d ,

$$\frac{\overline{\delta \epsilon}}{\epsilon_0} \simeq -2f_0 \simeq -2\Phi. \quad (3.32)$$

If the physical scale $\lambda_{\text{ph}} \sim 2\pi a/k$ is much smaller than the Hubble scale, i.e., $k\eta \gg 1$, we keep only the Δ term and obtain for the mode k

$$\frac{\overline{\delta \epsilon}}{\epsilon_0} \simeq \frac{\Delta}{6} \left(f_0\eta^2 + f_d \frac{1}{M_{\text{P}}^5 \eta^3} \right) \simeq -\frac{k^2}{6} \left(f_0\eta^2 + f_d \frac{1}{M_{\text{P}}^5 \eta^3} \right). \quad (3.33)$$

Then, one considers the oscillatory modes implied in Fig. 3.8, $\delta = \delta_{\mathbf{k}}(t)e^{i\mathbf{k}\cdot\mathbf{q}}$. It is shown in Fig. 3.9. The result is the same as that obtained in the Newtonian limit.

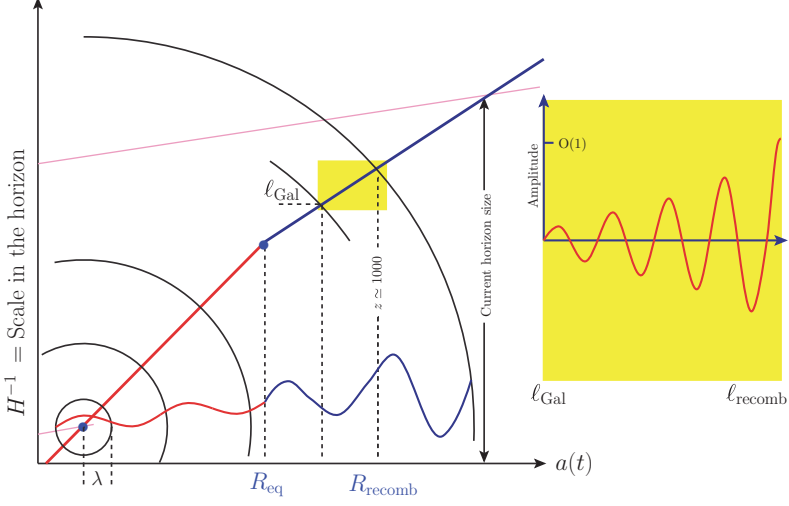


Fig. 3.9. An illustrative view of the scales of H^{-1} near the equality point of Fig. 1.3. The horizon after inflation is marked as the thick red line during radiation domination and the thick blue line during matter domination. The crossing point of the lavender line is the horizon scale. The sphere of R_{eq} is the one for “matter = radiation”, and R_{recomb} is the one at $z \simeq 1000$.

Since it is intuitive to present physics of $\delta_{\mathbf{k}}(t)$ in the Newtonian limit, we cite the equation written in the Newtonian limit,²

$$\ddot{\delta}_{\mathbf{k}} + 2H\dot{\delta}_{\mathbf{k}} + \left(\frac{c_s^2 k^2}{a^2} - \frac{1}{2} \frac{\epsilon_0}{M_{\text{P}}^2} \right) \delta_{\mathbf{k}} = 0, \quad (3.34)$$

where $\delta = \overline{\delta\epsilon}/\epsilon_0$,³ and a is the scale factor. The critical length scale is the Jeans length, determined by the vanishing last term,

$$\lambda_J^{\text{ph}} = \frac{2\pi a}{k_J} = 4\pi c_s \sqrt{\frac{M_{\text{P}}^2}{2\epsilon_0}}. \quad (3.35)$$

Here, λ^{ph} is the physical wavelength given by $\lambda^{\text{ph}} = a\lambda$. For this Jeans scale, the perturbation grows with instability. The beginning of this instability growth is right after the horizon crosses the quantum scale k_0 of Fig. 3.8. The point where the scale $\lambda = 2\pi/k_0$ enters into the horizon is shown as the small circle in Fig. 3.9. When the horizon expands much more to include many waves of wavelength λ , the situation is shown as the expanding circles. For example, this red colored wave oscillates with sound frequency. The size of inhomogeneity corresponding to λ is still λ . The quantum fluctuation includes all frequencies, i.e., all scales. The amplitudes for these different waves are assumed to be the same, which defines the universal

²It is given in [23, Eq. (6.47)].

³We do not need a gauge condition in the Newtonian limit, i.e., $\overline{\delta\epsilon} = \delta\epsilon$.

Harrison–Zeldovich spectrum [24]. Thus, as the horizon expands, larger and larger wavelengths are continuously entering into the horizon with the same strength of amplitude. Suppose that the galactic-scale wavelength ℓ_{Gal} enters into the horizon where k_0 of Fig. 3.8 now corresponds to $2\pi/\ell_{\text{Gal}} < \pi/R_{\text{eq}}$, i.e., the point is between R_{eq} and R_{recomb} in Fig. 3.9, which is shown more clearly in the inset. This is during the matter-dominated era. From then on, this galactic-scale wavelength oscillates as a stationary mode as in Fig. 3.8. It is said that the galactic scale is in the causal contact and CDM particles are attracted to this inhomogeneity δT_0^0 by the gravitational attraction. Since $\delta T_0^0 \ll$ (average matter energy), there are plenty of nearby CDM particles to reshuffle their relative density. This matter inhomogeneity follows the growth rate of δ shown as the blue curve in Fig. 3.9. When δ becomes order 1, it goes into a nonlinear regime and becomes a gravitationally bound structure. The gravitationally bound structures do not expand exponentially while the distances between the gravitationally bound structures expand exponentially. These gravitationally bound structures became galaxies. The sizes of galaxies are determined when δ becomes order 1, i.e., around the time of recombination, and the distances between galaxies are determined when the fluctuation size the time of recombination entered into horizon. This situation is illustrated in the upper figure of Fig. 3.10. When the CDM particles fall as shown with green lines, the inhomogeneity profile changes, i.e., δT_0^0 changes. This change also changes g_ν^μ and the scale of inhomogeneity may become somewhat smaller than the average distance between inhomogeneities as illustrated in the lower figure of Fig. 3.10. Roughly, at the time when this galactic scale goes into nonlinear regime, the temperature dropped to the recombination period. Then, baryons begin to decouple from photons and they fall into the gravitational potential and the galactic-scale stationary wave attracts baryons also. It is illustrated with red arrows in the lower figure of Fig. 3.10. Some of these baryons end at stars and shine, which are what we see starry galaxies in

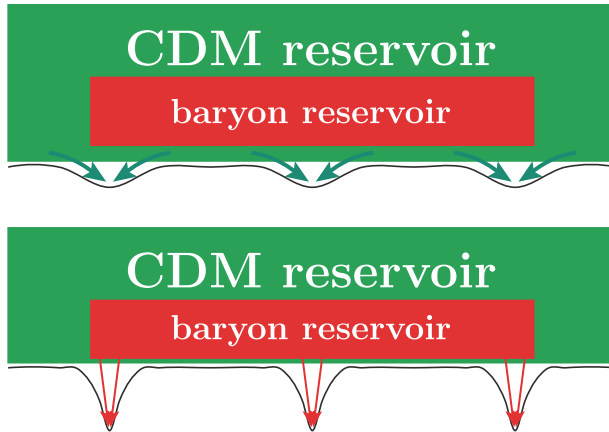


Fig. 3.10. Falling of matter particles in the gravitational potential well.

Table 3.1. Planck TT power spectra peak positions and amplitudes ($\propto \mathcal{D}_\ell$).

TT power	Position [ℓ]	Amplitude [μK^2]
1st peak	220.0 ± 0.5	5717 ± 35
2nd peak	537.5 ± 0.7	2582 ± 11
3rd peak	810.8 ± 0.7	2523 ± 10
4th peak	1120.9 ± 1.0	1237 ± 4
5th peak	1144.2 ± 1.1	797.1 ± 3.1
6th peak	1776 ± 5	377.4 ± 2.9
7th peak	2081 ± 25	214 ± 4
8th peak	2395 ± 24	105 ± 4

Fig. 3.6. Note that the scale ℓ_{Gal} is smaller than ℓ_{recomb} as mentioned above and the amplitude of the oscillation of the wavelength ℓ_{Gal} is $\mathcal{O}(1)$ at $z \simeq 1000$.

The scales for structures discussed above arise for all wavelengths. Namely, when the scale ℓ_{Gal} enters into the horizon, there are small-scale inhomogeneities $\ell < \ell_{\text{Gal}}$ inside ℓ_{Gal} . These smaller scale inhomogeneities all went into the nonlinear regime. So, inside ℓ_{Gal} , these small-scale inhomogeneities also (together with the CDM particles) reshuffle to satisfy the equation for δT_0^0 . At the time of recombination, the scales $\ell > \ell_{\text{Gal}}$ have not grown enough (i.e., they are not in the nonlinear regime yet) and baryons are not expected to fall into the gravitational potential well of the size $\ell > \ell_{\text{Gal}}$. This may be a reason that the galactic scale is the consequence of the existence of CDM.

The power spectra observed by the Planck satellite show eight TT correlation peaks, as shown in Table 3.1. The acoustic peaks in the ℓ reveal the underlying physics of oscillating sound waves in the coupled photon–baryon fluid, attracted by CDM potential perturbations. They enable the Planck group to estimate precisely the underlying cosmological parameters (the peak position ℓ and the amplitudes at the peaks) [25]. The eight acoustic peaks imply the scales where some noticeable interactions were applicable at the time of those scales entering into the horizon. One can think of important mass fractions of the Universe after CDM, i.e., that of baryons. Baryons gravitate after CDM, around the time of recombination epoch and a bit later. These can be distinguishable points in the era of primordial nucleosynthesis. The first was the formation of hydrogen i.e., the recombination era, when the CDM peak appeared. The next periods are at the times of forming deuteron (^2D), ^3He , ^4He , ^5Li , ^6Be , ^7Be , etc. Absence of a prominent peak after these can be used to give a bound on the sum of SM neutrino masses. But the best limit from Planck experiment came from gravitational lensing, $\sum_i m_{\nu_i} < 0.23\text{ eV}$ [10].

3.3. Simulation in the cosmos

Computational simulation physics has become a powerful tool for answering astrophysical questions. The N -body simulation technique has become the most powerful

tool for the study of evolution of astrophysical systems bound by the gravitational force: the solar system, star clusters, formation of elliptic galaxies, and the large-scale structure of the Universe. The ingredients of N bodies can be rocks, stars, or galaxies, depending on the limitation of the computing power and the structures to be investigated.

To trace the evolution of the CDM distribution, the N -body simulation studies under the gravitational force on the large-scale structures in the Universe [26, 27] are particularly relevant in this book. This is based on the hierarchical clustering scenario in the inflationary model. For the large-scale structure, the Friedmann–Lemaître–Robertson–Walker (FLRW) model in general relativity is used. In the simulation, N particles move according to the following $6N$ Newtonian differential equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}, \quad (3.36)$$

$$m \frac{d\mathbf{v}}{dt} = \mathbf{F}. \quad (3.37)$$

There are many issues to overcome to obtain a reasonable simulation. For example, the acceleration needs N^2 force terms (of N particles). They must be reduced to a smaller number of terms for a successful computation, for example, to $O(N \log N)$ terms. The Barnes–Hut algorithm [28] may be used for this purpose.

3.3.1. Scales of galaxies and beyond

Toward understanding the physical processes of building up the real galaxies, one gets an idea on suitable parameters in the simulation by comparing a simulation with observed surveys in the sky. According to the hierarchical clustering scenario discussed in Section 3.2.2, galaxies are assembled by merging and accretion of numerous lumps of different sizes and masses. There seem to be enough observed normal-sized galaxies to account for this distribution of the N -body simulation.

Recent galaxy redshift surveys on scales ranging from a few tens kpc to a few hundreds Mpc are a powerful tool for studying the recent history of the large-scale three-dimensional distribution of galaxies. The first runner Millennium simulation [26] used $N > 10^{10}$ particles in a cubic region of the Universe over 2×10^9 light-years on a side. A particle mass in the simulation is about $10^8 M_\odot$. In this way, the scientists of the Virgo consortium were able to recreate an evolutionary history of $10^{18} M_\odot$ or for the 20 million or so galaxies. There are also Bolshoi⁴ and MultiDark simulations [27]. The Bolshoi simulation took 6 million cpu hours to run on the Pleiades supercomputer at NASA Ames Research Center to calculate the evolution of a typical region of the Universe at 10^9 light-years across. Thus, the portions of the Universe studied at Millennium and Bolshoi simulations are similar.

⁴It means “great” or “grand” in Russian.

Color-selected surveys are used for studying larger scales. For example, the Baryon Oscillation Spectroscopic Survey (BOSS) tries to look for the scale of baryon acoustic oscillations (BAO) by studying the Lyman- α forest [29]. The survey Horizon Run 4 tried to compare the simulation at somewhat smaller scales than those of BOSS with the data on red galaxies [30].

A Horizon Run 4 simulation, which is not plagued by the dwarf galaxy problem, is shown in Fig. 3.11 which compared the simulation (b) with the HectoMAP survey (a) [31]. One may judge that the simulation is very similar to the observed survey.

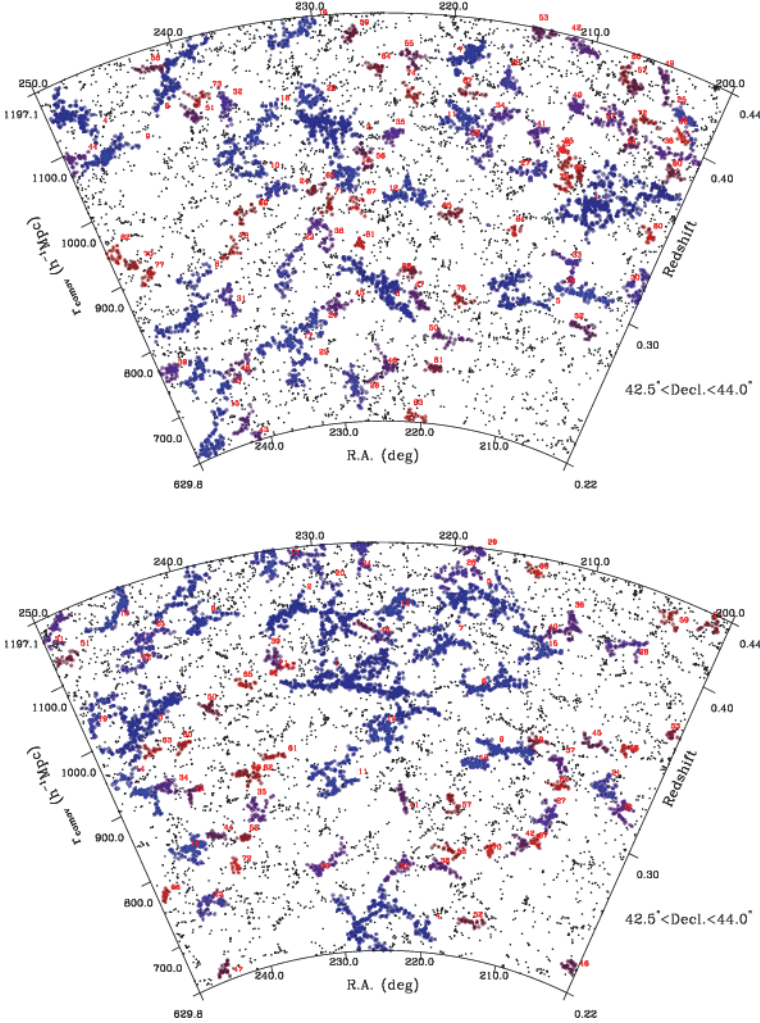


Fig. 3.11. Horizon Run 4 simulation: (*Upper figure*) the HectoMAP survey (Fig. 6 of [31]), and (*Lower figure*) Horizon Run 4 simulation with $\Omega_{\text{CDM}} = 0.9\Omega_m$ in the Λ CDM model (Fig. 9 of [31]).

This scale, larger than the cluster scale but ending around the BAO scale, is useful to study great walls and voids as emphasized in [31].

3.3.2. Subhalo scales

But, this process is not 100% efficient in destroying all of the accreted satellite galaxies. In fact, there are the satellite dwarf galaxies in Milky Way and M31. But, the observed number of satellites demand destroying most of the mass lumps with a few remaining. It was first observed in Ref. [32], where about 300 satellites inside a 1.5 Mpc radius were predicted by the N -body simulation while only about 40 satellites were observed in the Local Group. In the Milky Way, 500 satellites remained in the simulation while 11 were observed [33]. In other words, the N -body simulation is not effective in destroying satellite galaxies by a factor of 7 or more. This is a huge discrepancy and the problem is generally accepted, and there appeared the *missing satellite problem* or small-scale crises.

This has led to numerous studies on the unobservable small-scale DM clump scenarios below the galactic scale. It is called the dwarf galaxy problem.

3.4. Dwarf galaxy problem

The dwarf galaxy problem or the missing satellite problem has astrophysical and cosmological solutions. Figure 3.12 is an artistic view of 17 dwarf galaxies (a little bit more than 11 mentioned above) in the Milky Way.

The missing satellite problem could be solved by baryonic physics. Astrophysical solutions [34], related to baryonic physics, are based on the idea that the smaller halos do exist but only a few of them end up becoming visible as in Fig. 3.12 because they have not been able to attract enough baryonic matter to create a visible dwarf galaxy. The velocity threshold at which subhalo and dwarf satellite counts diverge is close to the $\sim 30 \text{ km s}^{-1}$ at which the heating of intergalactic gas by the ultraviolet photoionizing background should suppress gas accretion onto halos [36]. Thus, reionization could suppress the formation of dwarf galaxies by preventing low-mass DM halos from acquiring enough gas to form stars after $z \sim 10$ [38].

Another possibility is that the observed dwarf galaxies were once much more massive objects that have been later reduced to their present dwarf galaxies by complex interactions. But there is a question why baryons were more influenced than DM by this tidal stripping [39].

N -body simulations illustrate the missing satellite problem. For the projected DM density distribution of a $10^{12} M_{\odot}$ CDM halo, a cosmological N -body simulation is shown in Fig. 3.13 [35]. Because CDM preserves primordial fluctuations down to very small scales, halos today are filled with enormous numbers of subhalos that collapse at early times and preserve their identities after falling into larger systems.

The mass of DM in the central 0.3 kpc of the host subhalos is $M_{0.3} \approx 10^7 M_{\odot}$ across an enormous range of luminosities, $L \sim 10^3 - 10^7 L_{\odot}$ (encompassing the

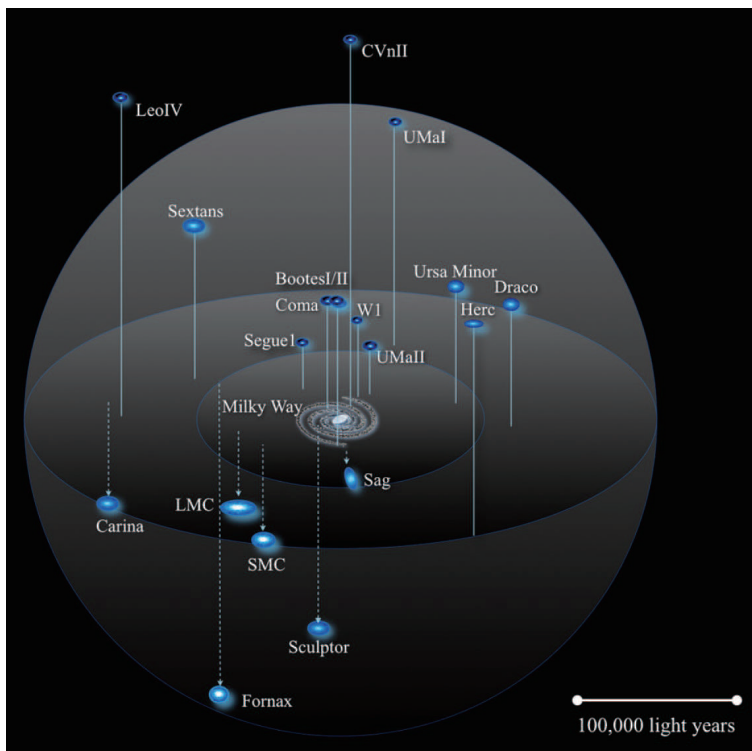


Fig. 3.12. An artistic view of dwarf galaxies in the Milky Way by J. S. Bullock, M. Geha and R. Powell [53]. Each dwarf contains up to several billion stars, compared to several hundred billion in the Milky Way.

classical dwarf spheroidal (dSph) as well as the SDSS dwarf [41]), is estimated from stellar dynamics. This suggests that the mapping between halo mass and luminosity becomes highly stochastic near this mass threshold [40]. Thus, recently, attention has focused on the most luminous satellites. Circles in Fig. 3.13 mark the nine most massive subhalos in the N -body simulation [35]. Then, one expects that Milky Way’s classical dwarf satellites host this kind of DM dense satellites, exceeding the mass inferred from stellar dynamics of observed dwarfs, by a factor ~ 5 [42, 43]. However, one notices dim satellites in Fig. 3.12 instead of this kind of bright DM-dominated satellites. Even though the degree of discrepancy varies with the particular realization of halo substructure and with the mass of the main halo, the discrepancy appears too large to be a statistical fluke even for a halo mass at the low end of estimates for the Milky Way. Reference [42] named this “too big to fail problem”.

The cosmological solutions include changing the power spectrum at small scales [44] or proposing DM as warm⁵ DM [45] or decaying DM [46]. Warm DM,

⁵“Warm” in the sense that the effect of its velocity dispersion on structure formation is not negligible. Particle physics candidates include the gravitino and sterile neutrinos. On the other hand, the “cold” DM effect of its velocity dispersion on structure formation is completely negligible.

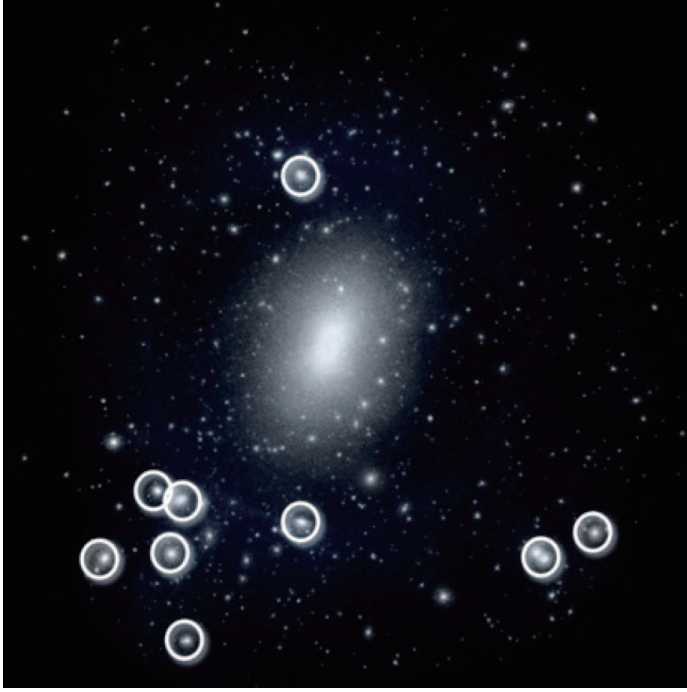


Fig. 3.13. High density satellites in an N -body simulation [35] and a too big-to-fail problem [37].

however, cannot give large cores to dSph galaxies while also being consistent with cosmological structure formation [47], i.e., warm DM cannot completely solve the small-scale crises, which is the *Catch 22 problem* of warm DM.

An ultra light axion (ULA) with mass $m_{\text{ULA}} \approx 10^{-22}$ eV making up a dominant ($\gtrsim 90$ %) component of the DM can provide large cores to dSph galaxies [48] (solving the “cusp–core” problem) and is consistent with both the CMB [49] and high- z galaxy formation [50], thus avoiding the Catch 22 problem of warm DM. The particle physics realization 10^{-22} eV axion is given in [51] and its importance is stressed in [52].

Exercise

1. For the Einstein tensor $G^\mu_\nu = \mathcal{R}^\mu_\nu - \frac{1}{2}\delta^\mu_\nu \mathcal{R}$, obtain the lowest order components

$${}^{(0)}G^0_0 = -\frac{3H^2}{a^2}, \quad {}^{(0)}G^0_i = 0, \quad {}^{(0)}G^i_j = -\frac{1}{a^2}(2H' + H^2)\delta^i_j, \quad (3.38)$$

where $H = a'/a$ is the Hubble parameter.

2. Show that

$$\overline{\delta T_0^0} = \delta T_0^0 - \left({}^{(0)}\delta T_0^0 \right)' (B - E'), \quad (3.39)$$

$$\overline{\delta T_i^0} = \delta T_i^0 - \left({}^{(0)}T_0^0 - \frac{1}{3} {}^{(0)}\sum_k T_k^k \right) (B - E')_{,i}, \quad (3.40)$$

$$\overline{\delta T_j^i} = \delta T_j^i - \left({}^{(0)}T_j^i \right)' (B - E'). \quad (3.41)$$

are gauge invariant.

3. If the energy–momentum tensor is diagonal, i.e., $T_j^i \propto \delta_j^i$, show that the modes in Eq. (3.14) gives $\phi = \psi$.

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Chapter 4

Symmetry Principles

What we observe is due to our method of questioning — W. Heisenberg

After the discovery of neutron in 1932, Fermi introduced four-fermion interactions of electron, electron-type neutrino, proton, and neutron. With Fermi's four-fermion interactions of 1934, there are 34 terms with 34 coupling constants. But, soon after the discovery of parity violation in weak interactions in 1956, it was established that the weak interaction was described by the four-fermion current–current interaction: the current of the form “ $V - A$ ” with one coupling constant published in [1, 2] and talked earlier in [3].¹

The “ $V - A$ ” current is an operator with dimension 3. Thus, the current–current interaction has a coupling constant of $1/(\text{mass})^2$, and the weak interactions in late 1950s were limited to tree-level calculations for the low energy phenomena. Of course, it was not possible to calculate the loop corrections since the current–current weak interaction was not a renormalizable theory. For strong interactions, Yukawa's pseudoscalar interaction of pions with nucleons, a renormalizable theory, was partially successful at low energy. But this pion–nucleon theory involves a large coupling constant $g_{\pi NN}^2/4\pi \sim 14.7$ which did not allow a perturbation expansion. In 1960s, there was a dream to search for a theory of strong interactions as beautiful as quantum electrodynamics (QED).

Modern particle theory is quantum field theory (QFT) which incorporates both quantum phenomena and special theory of relativity. Except the gravitational interaction, interactions of elementary particles are well described in modern particle theory [4]. At the root of strong interactions, there is quantum chromodynamics (QCD) which is an $SU(3)$ gauge theory and renormalizable as QED. The weak and electromagnetic interactions are described by the standard model (SM) of elementary

¹See R. E. Marshak's talk at “International Conference on 50 Years of Weak Interactions”, Racine, Wisconsin, May 29–June 1, 1984.

particles which is a spontaneously broken renormalizable $SU(2) \times U(1)$ gauge theory and allows that the intermediate vector bosons $W^\pm$ and Z^0 obtain mass. In the Universe at temperature much below the quantum gravity scale, i.e., much below the reduced Planck mass scale M_P , these elementary particle interactions are sufficient to describe the evolution of the Universe in the standard Big Bang cosmology.

String theory is a kind of theory with a potential of describing physics near the Planck scale and provides us good hints how a complete theory including gravity might look like at the string scale. String scale is considered to be somewhat below the Planck mass in the small-scale string theory [5] and much below the Planck mass in the large-scale string theory [6]. In the Universe evolution here, we concentrate on physics below the string scale in the small-scale string theory framework² (if such consideration is needed). Let us call this scale the grand unification theory (GUT) scale of elementary particles. The GUT scale is $M_{\text{GUT}} \approx 10^{16}$ GeV.

Particle cosmology describes the Universe in terms of elementary particles and their interactions. Therefore, it is of utmost importance to know what are the elementary particles below M_{GUT} . The information on elementary particles are contained in the quantum fields, $\phi(x), \psi(x)$, etc.³ The highest energy scale probed by high energy accelerators so far is the electroweak scale, $\gtrsim 100$ GeV, which is usually mentioned as a TeV scale. From high energy experiments, the particle content above the electroweak scale is not completely known at present. Thus, for the interactions of the SM particles, usually one takes the *bottom-up* approach where all possible interactions consistent with the SM symmetry are considered. However, any particle just above the TeV scale can affect the evolution of the Universe. To guess what particles are possible above the TeV scale, the *top-down* or *bottom-up* approach is taken depending on one's emphasis on the underlying assumptions.

Except the Einstein equation of spin-2 graviton, field equations of spin-0 fields are influential in discussing the Universe evolution. It is the Klein–Gordon equation,

$$(\partial_\mu \partial^\mu + m^2)\phi(x) + V'(\phi, \dots) = 0, \quad (4.1)$$

where m is the mass of the spin-0 particle and V' is the first derivative of the interaction Hamiltonian $V(\phi, \dots)$ with respect to ϕ . Equation (4.1) is written in the flat space and we must add the Hubble friction term $3H\dot{\phi}$ to discuss its evolution in the Universe as discussed in Chapter 2.

4.1. Quantum numbers

The basic operations in quantum mechanics are symmetry transformations. Thus, symmetry in the QFT description is the key concept in any theory on dark matter,

²Nevertheless, the large-scale string case is included in the low energy effective interactions.

³In most cases in this book, ϕ and ψ represent spin-0 and spin- $\frac{1}{2}$ fields, respectively.

either in the bottom-up approach or in the top-down approach, and theory on dark matter must be based on the symmetry principle.

Any operation in QFT is encoded in field operators. A Hermitian spin-0 field ϕ is Fourier-decomposed as

$$\phi(x) = \int \frac{d^3p}{(2\pi)^3 2E} [a(p)e^{-ip \cdot x} + a^\dagger(p)e^{ip \cdot x}], \quad (4.2)$$

where $p = Ex^0 - \mathbf{p} \cdot \mathbf{x}$, $a(p)$ is the annihilation operator of particle ϕ with momentum p and $a^\dagger(p)$ is the creation operator of momentum p . A complex spin-0 field is made of two Hermitian spin-0 fields. A complex 4-component spin- $\frac{1}{2}$ Dirac field is Fourier-decomposed as

$$\psi(x) = \sum_{s=+\frac{1}{2}, -\frac{1}{2}} \int \frac{d^3p}{(2\pi)^3 2E} [b(p, s)u(p, s)e^{-ip \cdot x} + d^\dagger(p, s)v(p, s)e^{ip \cdot x}], \quad (4.3)$$

where $b(p, s)$ is the annihilation operator of the fermion with momentum p and spin s , $d^\dagger(p, s)$ is the creation operator of the antifermion with momentum p and spin s , $u(p, s)$ and $v(p, s)$ are 4×1 column matrices called “Dirac spinors”. We can consider the dagger of ψ , i.e., $\bar{\psi} = \psi^\dagger \gamma^0$, where $\bar{\psi}$ contains $b^\dagger$ and d , i.e., creation and annihilation operators of the particle. In Eqs. (4.2) and (4.3), the spacetime symmetry operations act on the coordinate x , and the other (*internal*) symmetry operations act on $a, a^\dagger, b, b^\dagger, d$, and $d^\dagger$.

In Nature, symmetries are realized either in the Wigner–Weyl manner or in the Nambu–Goldstone manner.⁴ Therefore, we must consider dark matter possibilities in these two realizations.

Symmetries are broadly classified into two classes: discrete and continuous symmetries. A symmetry transformation can be parameterized by a real number α . If α takes only discrete values, the symmetry is called *discrete symmetry*. If α takes continuous values, the symmetry is called *continuous symmetry*. Quantum mechanics can be called “phase mechanics” because any transformation in quantum mechanics is represented by a unitary transformation, e.g., $\psi(x) \rightarrow e^{i\alpha} \psi(x)$, i.e., symmetry transformation in quantum mechanics involves phases. The transformation of the form e^α with a real parameter α , e.g., the scale transformation, is not considered in this book.

In Table 4.1, we present quantum numbers, or the charge eigenvalues of charge operators say Q , corresponding to several known symmetries in particle physics. If the Hamiltonian $\mathcal{H}$ is invariant under the symmetry transformation, the unitary transformation gives

$$e^{i\alpha Q} \mathcal{H} e^{-i\alpha Q} = \mathcal{H}, \quad \text{or} \quad e^{i\alpha Q} \mathcal{L} e^{-i\alpha Q} = \mathcal{L}. \quad (4.4)$$

⁴This distinction is applied usually in continuous symmetries.

Table 4.1. Several symmetries and conserved quantum numbers considered in modern particle physics. [Discrete and continuous symmetries are denoted as disc and cont, respectively.]

Transformation	disc/cont	quantum number (or eigenvalue)
scale change	cont	not considered here
space-displacement	cont	$\mathbf{p}$, momentum
time-displacement	cont	E , energy
spatial-rotation	cont	$\mathbf{J}$, angular momentum
space inversion	disc	P , parity; ± 1
rotation in isospin space	cont	I , isospin
charge conjugation	disc	$\mathcal{C}$, charge conj.; ± 1
G conjugation	disc	G , G parity; ± 1
gauge transform $U(1)_{\text{em}}$	cont	Q_{em} , electric charge
gauge transform $SU(3)_c$	cont	color charges
gauge transform $SU(2) \times U(1)$	cont	weak charges
global transform $U(1)_B$	cont	B , baryon number
global transform $U(1)_L$	cont	L , lepton number
permutation symmetry S_n	disc	S_n quantum number
anticommuting ϑ transform	cont	R charge in SUSY
parity related to ϑ in SUSY	disc	R parity in SUSY
even S_4 transform, A_4	disc	A_4 quantum number

A vector representing a particle state, in the linear vector space, can be created from the vacuum by applying a creation operator. For a fermionic particle, for example, we can represent a particle state of momentum $\mathbf{p}$ and spin- s as

$$|\mathbf{p}, s\rangle = b^\dagger(\mathbf{p}, s)|0\rangle, \quad (4.5)$$

and the quantum number of an operator Q of the state is q ,

$$Q|\mathbf{p}, s\rangle = q|\mathbf{p}, s\rangle, \quad (4.6)$$

where q is the eigenvalue of Q . When one says that Q is conserved, it means that the sum of all q 's is conserved. It also means that the lightest particle with some specific q is absolutely stable because one cannot make q as a sum of q 's of lighter particles. For example, if baryon number B is conserved, proton which is the lightest particle with $B = 1$ is absolutely stable. In addition to this conservation law, the symmetry realizations of Section 4.4 must be considered to list dark matter candidates.

Conservation of internal charges is described by continuity equations. The field equation of ϕ_i is given by the so-called Gell-Mann–Levy equation [7], assuming that $\mathcal{L}$ is a function of ϕ_i and $\partial^\mu \phi_i$ only,

$$\partial^\mu \frac{\delta \mathcal{L}}{\delta(\partial^\mu \phi)} = \frac{\delta \mathcal{L}}{\delta \phi}. \quad (4.7)$$

Charge conservation, corresponding to the symmetry Eq. (4.4), implies that the Lagrangian is invariant under some change of the field ϕ_i ,

$$\mathcal{L}(\phi_i + \delta \phi_i) - \mathcal{L}(\phi_i) = 0, \quad (4.8)$$

or

$$\begin{aligned} \frac{\delta \mathcal{L}}{\delta(\partial^\mu \phi_i)} \delta(\partial^\mu \phi_i) + \frac{\delta \mathcal{L}}{\delta \phi_i} \delta \phi_i &= \frac{\delta \mathcal{L}}{\delta(\partial^\mu \phi_i)} (\partial^\mu \delta \phi_i) + \partial^\mu \left(\frac{\delta \mathcal{L}}{\delta(\partial^\mu \phi)} \right) \delta \phi_i \\ &= \partial^\mu \left(\frac{\delta \mathcal{L}}{\delta(\partial^\mu \phi)} \delta \phi_i \right) = 0, \end{aligned} \quad (4.9)$$

from which we define a conserved current,

$$j_i^\mu = \frac{\delta \mathcal{L}}{\delta(\partial_\mu \phi)} \delta \phi_i. \quad (4.10)$$

For a continuous symmetry where the parameter can be infinitesimal, i.e., for a conserved current, the continuity equation (4.9) leads to “charge Q_i conservation” where Q_i is the spatial integral of j_i^0 ,

$$Q_i = \int d^3x j_i^0, \quad (4.11)$$

with

$$\dot{Q} = 0. \quad (4.12)$$

In Table 4.1, the quantum numbers for cont correspond to those of Eqs. (4.11) and (4.12). In this case, the unitary transformation corresponds to $U = e^{iQ_i \alpha_i}$.

For a discrete transformation, the unitary transformation itself is usually used for the quantum numbers in Table 4.1. Here again, the continuity equation is the basis for the conservation of discrete charges, with eigenvalues taking discrete values.

So far, spin-0 fields have been used for explicit illustrations. But the well-known matter fields are spin- $\frac{1}{2}$ Dirac fields given in (4.3). At a low energy scale compared to some heavy scale, the massless limit is a useful approximation. Hence, we begin the study from the massless limit of fermions.

4.1.1. *Majorana fermion*

The Dirac field (4.3) is complex and can have a phase quantum number. It can be B, L , or some others. If four independent components of a Dirac field are reduced to two independent components by constraints, the spin- $\frac{1}{2}$ field can be considered to be real, which is then the so-called *Majorana fermion*. Another way is to have two complex components, which defines a two-component *Weyl fermion*. A Weyl fermion can carry a U(1) charge. If the U(1) charge of the Dirac field ψ is q , the U(1) charge of its charge conjugated field ψ^c is $-q$, which can be shown by taking

the complex conjugation of the Dirac equation. Here,

$$\psi^c = C\psi^*, \quad C = i\gamma^2, \quad (4.13)$$

where we use the standard γ matrices in modern particle physics [4].⁵ In the Dirac spinor space, $C = i\gamma^2$ exchanges the particle and antiparticle.⁶ If particle is also antiparticle, then there is no definition of particle quantum number. This defines a Majorana spinor,

$$\psi_M = \psi_M^c. \quad (4.14)$$

ψ_M is a 4-component spinor, but Eq. (4.14) defines that its components are equivalent to be real.

4.1.2. Weyl fermion

One can reduce the independent degrees in the Dirac spinor by killing the left- or the right-chirality states. For a Dirac spinor in the Weyl representation [8], one has a Weyl spinor by killing the right-chirality ($\psi_R = \frac{1-\gamma_5}{2}\psi$) and keeping only the left-chirality

$$\psi_W = \psi_L = \frac{1+\gamma_5}{2}\psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \\ 0 \\ 0 \end{pmatrix}, \quad (4.15)$$

where

$$\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.16)$$

The Weyl representation is widely used in supersymmetry (SUSY) [8]. With the metric $\eta^{\mu\nu} = \text{diag}(-1, +1, +1, +1)$, the γ matrices are

$$\gamma^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \bar{\sigma}^\mu & 0 \end{pmatrix}, \quad \bar{\sigma}^0 = \sigma^0, \quad \bar{\sigma}^i = -\sigma^i, \quad (4.17)$$

where the Pauli σ matrices are

$$\sigma^0 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.18)$$

⁵They are the Bjorken–Drell γ matrices except γ_5 , i.e., $\gamma_5 = -\gamma_5^{\text{BD}}$.

⁶In the isospin space, $i\sigma_2$ exchanges the upper component $I_3 = a$ and the lower component $I_3 = -a$, i.e., exchanging positive and negative charges.

A Dirac spinor is composed of two Weyl spinors χ_1 and χ_2 ,

$$\psi_D = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}. \quad (4.19)$$

A Majorana spinor has the same number of components as that of a Weyl spinor. So, in terms of one Weyl spinor χ , a Majorana spinor can be represented as

$$\psi_M = \begin{pmatrix} \chi \\ \chi^* \end{pmatrix}. \quad (4.20)$$

Equation (4.20) shows that ψ_M have both left- and right-chirality states and a mass term

$$-\frac{m}{2}\psi_M^T\gamma^0\psi_M = m\chi^\dagger\chi, \quad (4.21)$$

where we used the Weyl γ matrices, Eq. (4.17).

4.1.3. Bjorken–Drell γ matrices

The conventional Bjorken–Drell γ matrices are

$$\gamma_{\text{BD}}^0 = -\tilde{\gamma}_{\text{BD}}^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \gamma_{\text{BD}}^i = \tilde{\gamma}_{\text{BD}}^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}, \quad (4.22)$$

which are related to the Weyl notation (4.17) by a unitary transformation,

$$\tilde{\gamma}_{\text{BD}}^\mu = X^\dagger \gamma_W X, \quad X = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \quad (4.23)$$

Note that γ_W is given in Eq. (4.17) and the parity operator on the Dirac spinor is conventionally taken as γ_{BD}^0 .

4.2. Discrete symmetries

The simplest discrete symmetry is $\mathbf{Z}_2$ symmetry $\psi(x) \rightarrow e^{i\pi}\psi(x)$, which does not depend on the spacetime parameter x . It is a kind of internal symmetry. An equally simple but acting on the spacetime point $(t, \mathbf{x})$ is the familiar *parity* symmetry P ,

$$P : (t, \mathbf{x}) \rightarrow (t, -\mathbf{x}). \quad (4.24)$$

Parity can be discussed by reflection on the mirror (with some rotation).

How a quantum field behaves under P determines the parity property of the quantum field. The parity operation on a scalar field ϕ is

$$P : \phi(t, \mathbf{x}) \rightarrow e^{i\alpha} \eta \phi(t, -\mathbf{x}), \quad (4.25)$$

where the phase $e^{i\alpha}$ is unobservable and usually taken to be 1, and η can take +1 or -1 since $P^2\phi(t, \mathbf{x})$ must return to itself. For a real neutral particle, η is the parity quantum number. The neutral pion has $\eta = -1$ and called *pseudoscalar* boson. The Brout–Englert–Higgs–Guralnik–Hagen–Kibble (BEHGHK) boson h has $\eta = +1$ and is a *scalar* boson.⁷ Other useful discrete symmetries considered in particle physics are parity, charge conjugation, time reversal,⁸ and permutation symmetries, as summarized in Table 4.1.

For $\mathbf{Z}_N$ symmetry, the field returns to the original value after operating the transformation N times,

$$\mathbf{Z}_N : \phi(x) \rightarrow e^{i\frac{2\pi}{N}} \phi(x), \quad (4.26)$$

where x is four-dimensional (4D) spacetime coordinate. In general, the unitary operator for a discrete symmetry can be expressed as

$$U_{\text{discrete}} = e^{i2\pi\alpha}, \quad (4.27)$$

where α is a rational number.

4.3. Continuous symmetries

The simplest continuous symmetry is a $U(1)$ symmetry. The unitary operator for $U(1)$ on a complex function can be expressed as

$$U_{\text{continuous}} = e^{i\delta\alpha}, \quad \text{with } \delta\alpha = \text{infinitesimal}. \quad (4.28)$$

Its generalization to N states can be expressed as

$$U^i(\delta\alpha) = \mathbf{1}_{N \times N} + iQ^i\delta\alpha^i, \quad (4.29)$$

where Q^i acts on an $N \times 1$ column vector. Depending on the nature of this $N \times 1$ column vector, the number of independent parameters α^i is determined in group theory. The infinitesimal transformation defines the charge operator Q^i which is called “generator” of the continuous transformation. Unitarity of U implies that the generators are Hermitian, $Q_i^\dagger = Q_i$. If there is only one parameter, the continuous symmetry is called $U(1)$ symmetry.

⁷For the BEHGHK boson [11–13], we will use the word “Higgs boson” in this book.

⁸It is equivalent to CP in QFT.

The group transformations expressible as Eq. (4.29) are called *classical groups*. In this form, the multiplicative group transformations can be studied equivalently by commutators of generators. If there are n independent unrelated parameters, or completely commuting n generators, it is called $U(1)^n$ symmetry.

4.3.1. Non-Abelian groups

We consider the non-Abelian groups, where the generators do not commute. If one cannot separate out a part of the set of generators which commute with all the remaining generators, the group is called a *simple group*. Mathematically, it is stated that “A group is simple if it has no invariant subgroups except the unit element”. The *dimension* or *order* of the simple group is the number of generators of the adjoint representation. According to “the fundamental theorem” proved by Lie and Engels [9], the structure of the group is completely specified by the commutation relations among the generators. So, the study of simple group is completed by the algebra of generators.

Most general matrix groups or classical groups are general linear groups $GL(N)$, and the associativity in the matrix multiplication laws is one condition for these matrix groups $GL(N)$. Groups not satisfying the associativity are called exceptional groups. Suppose that the generators of (4.29) are represented by $N \times N$ matrices. These belong to subgroups of $GL(N)$ with the smallest nontrivial representation N . If the unitarity condition $U^{-1} = U^\dagger$ is imposed, they form $U(N)$. If the orthogonality condition $O^{-1} = O^T$ is imposed, they form $O(N)$. There are five exceptional groups: G_2 , F_4 , E_6 , E_7 , and E_8 . Some classical groups contain subgroups which are exceptional groups, e.g., G_2 subgroup of $SO(7)$ [10].

In Table 4.2, we list simple groups distinguishing $O(N)$ by the roots in the Dynkin diagrams for $N =$ even or odd. The algebras of simple groups are represented by $A_n, B_n, C_n, D_n, G_2, F_4, E_6, E_7$, and E_8 . Except the group $SU(N)$, there is no gauge anomaly, which is emphasized by the star in the last column of Table 4.2. To cancel the non-Abelian gauge anomaly, therefore, $SU(N)$ needs at least two matter representations. We note that spinor representations of $Sp(2n)$, $SO(2n)$ and E_6 can have complex representations, which can be used for chiral fermions at low energy. Chiral fermions are the keys for obtaining massless fermions at the GUT scale. Most widely used representations for this purpose are **16** of $SO(10)$ and **27** of E_6 .

4.3.2. Global symmetry

If the parameter $\delta\alpha$ of a continuous symmetry defined in Eq. (4.29) is constant, it is called *global symmetry*. With the global symmetry, for example, if Adam in Seoul performs a continuous transformation $\delta\alpha$, Eve in Cape Town transforms by the same amount $\delta\alpha$.

Table 4.2. Simple groups with dimensions of the adjoint and fundamental representations. [The algebra of classical groups are shown inside the square brackets with ranks shown as the suffices. The star in the last column of $SU(N)$ shows that there are some complex representations which by itself cannot cancel the non-Abelian anomaly. Other groups having complex representations, $Sp(2n)$, $SO(2n+1)$ and E_6 , do not have the non-Abelian anomaly.]

Name	Dim. of Adj.	Fund.	Complex rep.
$SU(N)$, $[A_n, n = N - 1]$	$N^2 - 1, n(n + 2)$	N	Possible*
$Sp(2n)$, $[C_n]$	$n(2n + 1)$	$2n$	Possible
$SO(2n)$, $[D_n]$	$n(2n - 1)$	$2n$	Possible
$SO(2n + 1)$, $[B_n]$	$n(2n + 1)$	$2n + 1$	No
G_2	14	7	No
F_4	52	26	No
E_6	78	27	Possible
E_7	133	56	No
E_8	248	248	No

4.3.3. Local symmetry

If the parameter $\delta\alpha$ of a continuous symmetry defined in Eq. (4.29) depends on the spacetime point x , i.e., $\delta\alpha(x)$, it is called *local or gauge symmetry*. Under the local symmetry, if Adam in Seoul performs a continuous transformation $\delta\alpha$, Eve in Cape Town need not transform by the same amount.

4.4. Realization of symmetries

Even if laws of physics admit some symmetries, their realization may not respect the symmetries of the laws.⁹ In this regard, an unfaithful symmetry widely mentioned is the *Heisenberg ferromagnet*. Magnetic moments $\vec{\mu}$ of atoms have three-dimensional directions. The law for ferromagnet satisfies the $O(3)$ symmetry, e.g., for the nearest neighbor interaction $\vec{\mu}_i \cdot \vec{\mu}_{(\text{neighbors of } i)}$, it is $O(3)$ -invariant, which is used in the Heisenberg Lagrangian. But, in Nature, we find ferromagnets which have certain magnetized directions, breaking the $O(3)$ symmetry. We interpret this phenomenon as, “the $O(3)$ symmetry has been broken in the course of the Universe evolution”. It is a kind of *spontaneous symmetry breaking*.

4.4.1. Discrete symmetries

Consider the following potential of a real scalar field ρ :

$$V(\rho) = \frac{\lambda}{4} (\rho^2 - v^2)^2, \quad \lambda > 0, \quad (4.30)$$

⁹Only in this section and Section 4.6 where particle physics terminology is used, we use the conventional particle physics notation [4], $\eta^{\mu\nu} = \text{diag}(+1, -1, -1, -1)$.

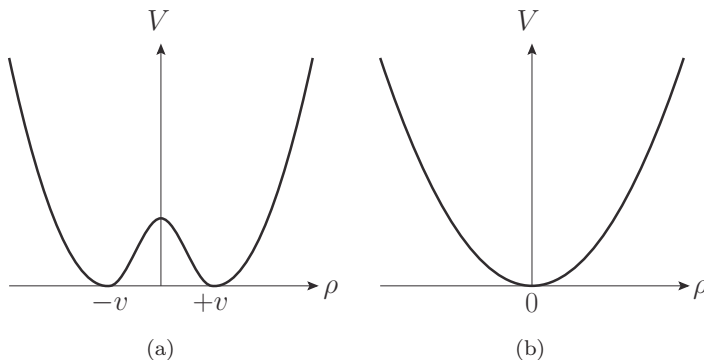


Fig. 4.1. (a) A potential with parity symmetry, $\rho \leftrightarrow -\rho$. (b) If $v = 0$, $\rho = 0$ is the only minimum.

which is depicted in Fig. 4.1(a). It has a parity symmetry, $+\rho \leftrightarrow -\rho$ for any real number v . Two vacua are at $\rho = \pm v$ ($v > 0$). If we choose one vacuum, say $\rho = +v$, the parity symmetry is spontaneously broken. On the other hand, if $v = 0$ in Eq. (4.30), viz. Fig. 4.1(b), then the potential has only one minimum at $\rho = 0$, i.e., it is unique and the parity symmetry of V is not broken at $\rho = 0$. Other discrete symmetries show a similar behavior.

4.4.2. Continuous symmetries

As discussed in Section 4.1, for a continuous symmetry, the conserved Nöther current is given by

$$J_\mu^a(x) = \frac{\delta \mathcal{L}}{\delta(\partial^\mu \phi)} \frac{\delta \phi}{\delta \alpha^a}, \quad (4.31)$$

where $\delta \phi = F_a \delta \alpha^a$ with the generator F_a of the symmetry operation and α^a is the parameter for the continuous symmetry transformation. The above symmetry is the symmetry obeyed by the Lagrangian, i.e., by the equations of motion. Nature assumes some continuous symmetry in the Lagrangian. One fundamental question is

“Can a physical state break the symmetry of the Lagrangian or not?”

It was known that negative answers to the above question also happen in Nature. One example for the negative realization is that we human beings are not left–right symmetrical. Of course, the parity is explicitly broken in the weak interaction Lagrangian, but the question on the life forms might not have used the weak interaction for the realization of the parity symmetry. Then, the left–right asymmetrical human being shows the broken parity. It is the evolutionary chance, probably from the time of the formation stage of DNA molecules in the Universe history. So, the asymmetry in the life forms with parity symmetric interactions is simply the evolutionary chance in the long history of the Universe, i.e., the planet Earth encodes the history of left–right symmetry breaking. Another example is the aforementioned

magnets. The electromagnetic interaction conserves the $SO(3)$ rotation symmetry, which is the symmetry of rotations in three space dimensions. If particles, especially the atoms, interact electromagnetically, they must preserve the rotational symmetry. But there exist natural magnets, which imply that the magnetized material breaks the rotational symmetry. These examples show that the realization of the symmetries of Lagrangian can be either preserved or broken in Nature.

In particle physics, the symmetry realization is specified in terms of the particle states, the states on which operators act in the Fock space. The realization starts with the vacuum $|0\rangle$, and on this vacuum, one creates one particle states, two particle states, etc. Since the multiparticle states are obtained by operating the particle creation operators, the symmetry realization mainly starts from that of the vacuum. Hence, the symmetry realization is classified as follows.

(i) Wigner–Weyl realization: The physical states respect the symmetry group, namely, the particle spectrum forms a *representation basis* of the continuous group. In particular, the vacuum is invariant, i.e., it is a singlet under the symmetry transformation (What else can it be?). In this case, since the states are the representations of the group, the symmetry operation on the states is well defined and unitarily implementable. This unitary transformation operator is generated by the charge operator,

$$Q^a = \int d^3x J_0^a(x), \quad (4.32)$$

which annihilates the vacuum,

$$Q^a|0\rangle = 0. \quad (4.33)$$

(ii) Nambu–Goldstone realization: The physical states do not form the representation basis of the symmetry group, and the vacuum state is degenerate (the only other alternative to the singlet). In this case, the charge is not well defined because the states are not representations of the symmetry group.

Suppose that we define the charge as (4.32). If the charge is well defined, we can consider the norm of the state $Q|0\rangle$,

$$\langle 0|QQ|0\rangle = \int d^3x \langle 0|j^0(x)Q|0\rangle = \int d^3x \langle 0|j^0(0)Q|0\rangle, \quad (4.34)$$

where the translational invariance obeyed by the vacuum, $e^{-iP_\mu a^\mu}|0\rangle = |0\rangle$, and the commutativity of P_μ and Q are used in the last equality. Since $Q|0\rangle \neq 0$ is assumed for the Nambu–Goldstone realization, we expect

$$\langle 0|QQ|0\rangle = \infty, \quad (4.35)$$

namely, the state $Q|0\rangle$ does not belong to a set of normalizable state, i.e., it does not belong to the Hilbert space we define for the Fock space. The inconsistency of the above argument can be traced back to the definition of Q . Thus, Q is not definable.

On the other hand, there appears a massless boson, the so-called *Goldstone boson*, which is shown below.

A Lagrangian for a massless real spin-0 boson φ is

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \varphi)^2 - \frac{1}{2}m^2 \varphi^2 \quad (4.36)$$

with $m^2 = 0$. But we will keep m^2 for a moment for a transparent discussion. Take the vacuum expectation value (VEV) of Eq. (4.36),

$$\begin{aligned} \langle 0 | (\partial^2 - m^2) \varphi(x) | 0 \rangle &= (\partial^2 - m^2) \langle 0 | \varphi(x) | 0 \rangle \\ &= (\partial^2 - m^2) \langle 0 | \varphi(0) | 0 \rangle = -m^2 \langle 0 | \varphi(0) | 0 \rangle = 0 \end{aligned}$$

where we have used the translational invariance. Therefore, we have either $\langle 0 | \varphi(0) | 0 \rangle = 0$ (the Wigner–Weyl realization) or $m^2 = 0$ for the case $\langle 0 | \varphi(0) | 0 \rangle \neq 0$ (the Nambu–Goldstone realization). Namely, the spin-0 field φ must be massless if its VEV is nonzero. In other words, a noninteracting theory (4.36) with $m^2 = 0$ has a continuous symmetry which is spontaneously broken. In this case, the continuous symmetry is the translation of the field itself

$$\varphi(x) \longrightarrow \varphi(x) + \lambda, \quad (4.37)$$

where λ is a continuous parameter. Note that from (4.37) $\langle 0 | \varphi(x) | 0 \rangle \neq 0$. Even if one introduces interactions, the appearance of the Goldstone boson is proved to exist which we will show below. The massless field we introduced is the Goldstone boson itself, and we say that the symmetry is nonlinearly realized as shown in (4.37). For the linear representation, the Goldstone boson field is exponentiated. If the Goldstone boson is a pseudoscalar field, the Goldstone boson is a phase field. However, a scalar Goldstone field, such as a dilaton, cannot be raised to a phase field.

For the simplest interacting fields with a continuous symmetry, consider two real spin zero fields ϕ_1 and ϕ_2 with the Lagrangian,

$$\mathcal{L} = \frac{1}{2} [(\partial_\mu \phi_1)^2 + (\partial_\mu \phi_2)^2] - V(\phi_1^2, \phi_2^2), \quad (4.38)$$

where we imposed a discrete symmetry $\phi_1 \rightarrow -\phi_1$ and $\phi_2 \rightarrow -\phi_2$ to give

$$V(\phi_1, \phi_2) = \frac{1}{2} m_1^2 \phi_1^2 + \frac{1}{2} m_2^2 \phi_2^2 + \lambda_1 \phi_1^4 + \lambda_{12} \phi_1^2 \phi_2^2 + \lambda_2 \phi_2^4. \quad (4.39)$$

The (00) component of energy–momentum tensor is $-\mathcal{L} + \sum_a \pi_a^0 \partial_0 \phi_a + \partial_\mu [F^\mu]$ with $\pi_a^0 = \partial^0 \phi_a$. F^μ is related by canonical transformations. Neglecting F^μ , we have

$$\begin{aligned} T^{00} &= \frac{1}{2} \sum_{a=1}^2 \left\{ \sum_{i=1}^3 (\partial^i \phi_a)^2 + (\partial^0 \phi_a)^2 + m_a^2 \phi_a^2 \right\} \\ &\quad + \lambda_1 \phi_1^4 + \lambda_{12} \phi_1^2 \phi_2^2 + \lambda_2 \phi_2^4. \end{aligned} \quad (4.40)$$

For $\lambda_1 > 0, \lambda_2 > 0$, and $\lambda_1 \lambda_2 \geq \frac{\lambda_1^2}{4}$, T^{00} is bounded from below. If $V = 0$ (i.e., with no interaction), one can construct many conserved currents. One of them is

$$J_{12}^\mu = \phi_1 \partial^\mu \phi_2 - (\partial^\mu \phi_1) \phi_2. \quad (4.41)$$

We can make J_{12}^μ conserved even with interaction V if it is a function of $\phi_1^2 + \phi_2^2$ only. In this case, of course two masses are identical. Note that the combination $\phi_1^2 + \phi_2^2$ is invariant under the transformation

$$\begin{aligned} \phi_1 &\rightarrow \cos \alpha \phi_1 + \sin \alpha \phi_2, \\ \phi_2 &\rightarrow -\sin \alpha \phi_1 + \cos \alpha \phi_2, \end{aligned} \quad (4.42)$$

which describes the symmetry $O(2)$. Under $O(2)$, ϕ_1 and ϕ_2 are grouped into a doublet

$$\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}. \quad (4.43)$$

In $O(2)$, there is only one Casimir invariant, $\phi_1^2 + \phi_2^2$, because the rank of $O(2)$ is 1. Thus, we can take a renormalizable potential as

$$V(\phi_1^2, \phi_2^2) = \frac{m^2}{2}(\phi_1^2 + \phi_2^2) + \frac{\lambda}{4}(\phi_1^2 + \phi_2^2)^2. \quad (4.44)$$

Introducing a complex field ϕ via

$$\phi \equiv \frac{1}{\sqrt{2}}(\phi_1 + i\phi_2), \quad \phi^* \equiv \frac{1}{\sqrt{2}}(\phi_1 - i\phi_2), \quad (4.45)$$

the Lagrangian can be written as

$$\mathcal{L} = (\partial_\mu \phi)^* (\partial^\mu \phi) - V[\phi^* \phi], \quad (4.46)$$

where

$$V[\phi^* \phi] = m^2 |\phi|^2 + \lambda |\phi|^4. \quad (4.47)$$

The Lagrangian (4.46) has a continuous symmetry,

$$\phi \longrightarrow e^{i\alpha} \phi, \quad \phi^* \longrightarrow e^{-i\alpha} \phi^*, \quad (4.48)$$

which is the $U(1)$ symmetry. Both $O(2)$ and $U(1)$ symmetries have one parameter of transformation and they have the same Lagrangian. They are isomorphic. Let us consider the case with $\lambda > 0$ so that the potential is bounded from below. The Hamiltonian density T^{00} is given by

$$\mathcal{H} = |\partial^0 \phi|^2 + |\partial^i \phi|^2 + V(|\phi|). \quad (4.49)$$

The lowest energy state with a constant field configuration in time and space appears. The constant scalar field, $\phi(x) = \text{constant}$, is called the classical field ϕ_c . Then, the potential $V(|\phi_c|)$ can behave as in Figs. 4.2 or 4.3.

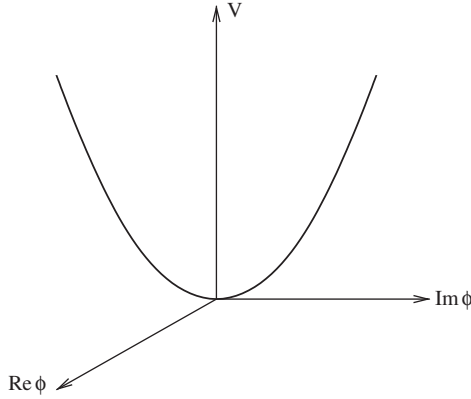


Fig. 4.2. The U(1) invariant potential.

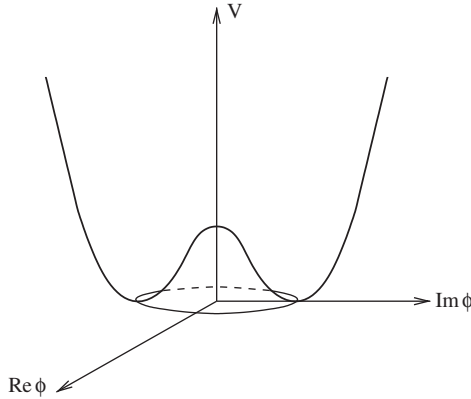


Fig. 4.3. The U(1) breaking potential.

For a positive m^2 , Fig. 4.2, the classical vacuum state at $\phi_c = 0$ is a singlet. Of course, a quantum state is obtained by quantizing the theory around this classical vacuum $\phi_c = 0$. It realizes the U(1) symmetry with the singlet vacuum in the Wigner–Weyl realization.

On the other hand, for $m^2 = -\mu^2 < 0$ of Fig. 4.3, the classical vacuum state is degenerate and must correspond to the Nambu–Goldstone realization. These degenerate vacua are not at $\phi_c = 0$, but at

$$\phi_c \equiv \langle 0 | \phi | 0 \rangle = \frac{v}{\sqrt{2}} e^{i\alpha} = \sqrt{\frac{\mu^2}{2\lambda}} e^{i\alpha}. \quad (4.50)$$

This vacuum degeneracy is parameterized by a continuous parameter α in Eq. (4.50). The number of continuous parameters depends on the symmetry we consider and how it is broken. In the present case, the U(1) symmetry has one parameter of

transformation and a nonvanishing value $\phi_c \neq 0$ for the classical field breaks it completely and hence the vacuum has one continuous parameter α for the degeneracy. Therefore, a transformation from one vacuum to another does not cost any energy, and we anticipate that there appears a massless excitation. A proper quantization must be around this degenerate vacuum, thus let us define the small perturbation of the quantum field ϕ' around this vacuum. Choose, for example without loss of generality, a point $\alpha = 0$ such that $\langle 0 | \text{Re } \phi | 0 \rangle = v/\sqrt{2}$ and $\langle 0 | \text{Im } \phi | 0 \rangle = 0$ as

$$\phi' = \phi - \langle 0 | \phi | 0 \rangle = \phi - \frac{v}{\sqrt{2}}, \quad (4.51)$$

which is equivalent to choosing $\phi = (1/\sqrt{2})(v + \text{Re } \phi' + i \text{Im } \phi')$. By exponentiating it, we have

$$\phi = \frac{1}{\sqrt{2}}(v + \rho)e^{ia/v}, \quad (4.52)$$

where $\rho = \text{Re } \phi'$ and $a = \text{Im } \phi'$. Now, the Lagrangian becomes

$$\mathcal{L} = \frac{1}{2} \{ (\partial_\mu \rho)^2 - 2\mu^2 \rho^2 + (\partial_\mu a)^2 \} - \lambda v \rho^3 - \frac{\lambda}{4} \rho^4 + \frac{1}{4} \mu^2 v^2. \quad (4.53)$$

The Lagrangian (4.53) describes two real fields ρ and a . The radial field ρ has the squared mass of $2\mu^2$ and the transverse direction (the circle at the minima in Fig. 4.3) or the phase field a has zero mass. This phase field a is called the Goldstone boson which arises from the breaking of U(1) global symmetry. This phenomenon that the vacuum breaks the symmetry is called the *spontaneous symmetry breaking*.¹⁰ Here, the appearance of Goldstone boson has been shown even in the interacting theory with the $\lambda|\phi|^4$ term. It appears as if under the U(1) transformation, a vacuum rotates to another vacuum on the degenerate circle of Fig. 4.3. In the spontaneously broken case, one does not define the charge, but the degenerate states are related by the phase transformation, which is related to the original U(1) transformation of the quantum field $\phi \rightarrow e^{i\alpha Q} \phi$, through a rotation of the classical (or vacuum) field,

$$\phi_c \longrightarrow e^{i\alpha} \phi_c. \quad (4.54)$$

The above transformation is equivalent to a shift of a ,

$$a \longrightarrow a + \alpha v, \quad (4.55)$$

which is the nonlinear transformation we considered in the free case. The spontaneously broken U(1) symmetry is equivalent to the field a having the shift symmetry

¹⁰It is called “spontaneous” because no external force is applied.

(4.55). In terms of a , the total charge in the volume V is

$$Q_V = \int_V d^3x \partial^0 a. \quad (4.56)$$

We would not have the inconsistency if the vacuum is degenerate since the infinity we obtained in Eq. (4.35) is from the assumption of a singlet vacuum. The normalizable state in the degenerate case can be obtained by identifying states related by the shift symmetry, and the infinity in Eq. (4.35) is due to this degree of degeneracy. As far as we keep this in mind, we can consider the charge generator (4.56) even in spontaneously broken cases by considering the finite region of the angular integral (angle from 0 to 2π) in Eq. (4.56).

The state $e^{i\theta Q_V}|0\rangle$ is one of the degenerate vacua which is different from the original one by the superposition of zero energy states of Goldstone boson a , but has the same energy as the original one. Since the vacuum is not a singlet, we have

$$Q_V|0\rangle \neq 0. \quad (4.57)$$

The last term in (4.53) is a constant which does not affect any particle physics dynamics. However, this term contributes to the gravitational interaction as a cosmological constant term Λ in Einstein's equation

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = 8\pi G_N T_{\mu\nu} + \Lambda g_{\mu\nu}, \quad (4.58)$$

which is derived from the action

$$S = \int d^4x \sqrt{g} \left[\frac{R}{16\pi G_N} - \frac{\Lambda}{8\pi G_N} + \mathcal{L}_{\text{PP}} \right], \quad (4.59)$$

where $\mathcal{L}_{\text{PP}}$ is the particle physics Lagrangian. Therefore, the vacuum energy in any Lagrangian is equivalent to the cosmological constant. Because the upper bound of the vacuum energy is about $(0.003 \text{ eV})^4$, one has to fine-tune the potential of Fig. 4.3 extremely well, one out of 10^{120} . This is a kind of naturalness problem, the so-called *cosmological constant problem*.

Non-Abelian group

Let us trivially generalize this to $U(1)^N$. There are N parameters describing the $U(1)^N$ transformation. If $U(1)^M$ ($M \leq N$) is broken, we can see that there appear M Goldstone bosons. Now, if the N parameter transformations are related, the symmetry group can be enlarged to a non-Abelian case. Consider an N parameter non-Abelian group G with generators T_a ($a = 1, 2, \dots, N$). Then, a quantum field ϕ

transforms under the group rotation to

$$\phi \longrightarrow e^{iT_a \omega^a} \phi, \quad (4.60)$$

where ω^a are the real angles denoting the amount of rotation in G . The supposed symmetry implies that the potential is invariant under the transformation

$$V(e^{iT_a \omega^a} \phi) = V(\phi), \quad (4.61)$$

which is useful to study the operation of generators on the vacuum. Consider the case that the minimum of V is *not a singlet* of the group G . But the vacuum is a singlet under H a subgroup of G . Let the elements of H be described by M parameters. The generators of H are well defined and annihilate the vacuum

$$T_a|0\rangle = 0 \quad \text{for } a = 1, 2, \dots, M. \quad (4.62)$$

But for the remaining parameters of transformation of G , the vacuum is not invariant,

$$T_a|0\rangle \neq 0 \quad \text{for } a = M + 1, \dots, N. \quad (4.63)$$

The parameters corresponding to the broken generators of (4.63) become the Goldstone boson, i.e., there appear $(N-M)$ Goldstone bosons with the quantum numbers (under H) identical to those of the broken generators.

As an example, consider an orthogonal group $O(N)$ with a fundamental representation

$$\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{pmatrix} \quad (4.64)$$

and its VEV given by

$$\langle 0|\phi|0\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ v \end{pmatrix}. \quad (4.65)$$

Even if the VEV is of the form $(v_1, v_2, \dots, v_n)$, we can change it by an $O(N)$ transformation to the form (4.65). In other words, these entries for VEVs can be obtained

by an $O(N)$ transformation on the VEVs we considered. Therefore, without loss of generality, the classical field can be expressed as

$$\phi = e^{ia_i T_i/v} \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ (\phi_1^2 + \phi_2^2 + \cdots + \phi_N^2)^{1/2} \end{pmatrix} = e^{ia_i T_i/v} \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ v + \rho \end{pmatrix}. \quad (4.66)$$

4.4.3. Loophole and BEHGHK mechanism

The Goldstone theorem has a loophole [14]. Here, we follow the discussion on the Goldstone theorem and its loophole presented in Ref. [31].

To show the appearance of the Goldstone boson(s), we started from a continuous symmetry, or a conserved current,

$$\partial^\mu J_\mu^a = 0. \quad (4.67)$$

For any function $F(y)$ constructed of field operators, consider its variation under a group transformation at the equal time

$$\delta F_b(y) \equiv F_b(y)' - F_b(y) = i\omega^a \int d^3x [F_b(y), J_a^0(x)]_{y^0=x^0}. \quad (4.68)$$

If the charge operator $Q_a = \int d^3x J_a^0(x)$ exists, this definition is the usual one, $\delta F(y) = i\omega^a [F(y), Q_a]$, where we considered the infinitesimal transformation on the state $F_b|0\rangle$. Suppose that the VEV of $\delta F(y)$ is nonzero,

$$\langle 0 | \delta F_b(y) | 0 \rangle = i\omega^a \int d^3x \langle 0 | [F_b(y), J_a^0(x)]_{x^0=y^0} | 0 \rangle \neq 0. \quad (4.69)$$

Observe that this quantity would be vanishing if the symmetry is unbroken. Therefore, Eq. (4.69) for the nonzero VEV of $\delta F(y)$ corresponds to a broken symmetry case. On the other hand, using the current conservation, we have

$$\int d^3x [F_b(y), \partial^\mu J_\mu^a(x)]_{x^0=y^0} = 0, \quad (4.70)$$

or

$$\frac{\partial}{\partial x^0} \int d^3x [F_b(y), J_a^0(x)] = - \int_V d^3x [F_b(y), \vec{\nabla} \cdot \vec{J}_a(x)] = - \int_\Sigma d\vec{\sigma} \cdot [F_b(y), \vec{J}_a(x)], \quad (4.71)$$

where Σ is the enclosing surface of V . If the RHS of (4.71) vanishes, i.e., the surface term vanishes, the quantity given in (4.69) is independent of time x^0 , and we can

remove the condition $x^0 = y^0$,

$$\langle 0 | \delta F_b(y) | 0 \rangle = i\omega^a \int d^3x \langle 0 | [F_b(y), J_a^0(x)] | 0 \rangle \neq 0. \quad (4.72)$$

Let us insert a complete set of eigenstates of P^μ , $\sum_n |n\rangle\langle n|$, in Eq. (4.72), and use the translational invariance

$$F_b(y) = e^{iP \cdot y} F_b(0) e^{-iP \cdot y}, \quad J_a^0(x) = e^{iP \cdot x} J_a^0(0) e^{-iP \cdot x}$$

to obtain

$$\begin{aligned} \langle 0 | \delta F_b(y) | 0 \rangle &= i\omega^a \sum_n \int d^3x \{ e^{iP_n \cdot (x-y)} \langle 0 | F_b(0) | n \rangle \langle n | J_a^0(0) | 0 \rangle \\ &\quad - e^{-iP_n \cdot (x-y)} \langle 0 | J_a^0(0) | n \rangle \langle n | F_b(0) | 0 \rangle \} \\ &= i\omega^a \sum_n (2\pi)^3 \delta^{(3)}(\mathbf{P}_n) \{ e^{iP_n^0(x_0-y_0)} \langle 0 | F_b(0) | n \rangle \langle n | J_a^0(0) | 0 \rangle \\ &\quad - e^{-iP_n^0(x_0-y_0)} \langle 0 | J_a^0(0) | n \rangle \langle n | F_b(0) | 0 \rangle \} \neq 0. \end{aligned} \quad (4.73)$$

Since Eq. (4.73) is independent of x^0 , the derivative with respect to x^0 should vanish:

$$\begin{aligned} &-\omega^a \sum_n (2\pi)^3 \delta^{(3)}(\mathbf{P}_n) P_n^0 \{ e^{iP_n^0(x_0-y_0)} \langle 0 | F_b(0) | n \rangle \langle n | J_a^0(0) | 0 \rangle \\ &\quad + e^{-iP_n^0(x_0-y_0)} \langle 0 | J_a^0(0) | n \rangle \langle n | F_b(0) | 0 \rangle \} = 0, \end{aligned} \quad (4.74)$$

where the quantity inside the curly bracket is nonvanishing since Eq. (4.73) is nonzero. Therefore, Eq. (4.74) is satisfied only if there exists a state with $P_n^0 = E_n = 0$ for $\mathbf{P}_n = 0$. This state $|n\rangle$ describes a state with zero mass

$$m_n^2 = E_n^2 - \mathbf{P}_n^2 = 0, \quad (4.75)$$

which is the Goldstone boson that we are discussing.

Higgs mechanism

Note that in the above proof, we have assumed the following:

- the vanishing surface term in Eq. (4.71),
- $\langle 0 | J_a^0(0) | n \rangle \neq 0$, and
- $\langle 0 | F_b(0) | n \rangle \neq 0$.

Note further that we derived the theorem when J_a and F_b do not annihilate the state $|n\rangle$, which show that the Goldstone boson state has the same quantum number as the broken generator corresponding to $\int J_a^{0\dagger}(x) d^3x$ which we stated in the previous section.

Now, let us scrutinize the assumption on the vanishing surface term more closely [14]. This condition is

$$\int_{\Sigma} d\vec{\sigma}_x \cdot [F_b(y), \vec{J}_a(x)] = 0 \quad (4.76)$$

at the surface Σ , enclosing the large volume V . The condition (4.76) is satisfied for a short range force, i.e., for a localized $\vec{J}_a(x)$, and also in a manifestly covariant theory. The well-known example for the local interaction is the nearest neighbor interaction in the Heisenberg ferromagnet. In a manifestly covariant theory, for $F(y)$, we can always choose a large volume V such that its boundary Σ is outside the lightcone from y and hence the commutator must vanish due to the causality condition. The field theory examples we considered before for the global $O(2)$ or $U(1)$ are manifestly covariant theories, and hence there appears the Goldstone boson. On the other hand, there do exist relativistic theories which do not have the manifest covariance: i.e., the gauge theories. In the radiation gauge where only physical particles appear, the gauge condition is

$$\vec{\nabla} \cdot \vec{A} = 0 \quad (4.77)$$

which does not show a manifest covariance. Therefore, one can anticipate that the Goldstone boson may not appear in gauge theories when the gauge symmetry is spontaneously broken. Indeed, it was shown to be the case and this phenomenon is called the BEHGHK mechanism [11–13].¹¹

The generalization of a global symmetry to a local symmetry such as the gauge theories is to make the parameter of transformation α spacetime-dependent $\alpha(x)$. We have considered the $U(1)$ global symmetry and non-Abelian global symmetry before. For a brief discussion on the Higgs mechanism, now let us consider a $U(1)$ gauge symmetry. A complex scalar field $\phi(x)$ transforms nontrivially under the $U(1)$ gauge transformation,

$$\begin{aligned} \phi &\longrightarrow e^{i\alpha(x)}\phi, \\ \phi^* &\longrightarrow e^{-i\alpha(x)}\phi^*. \end{aligned}$$

The kinetic energy term,

$$D_\mu \phi^* D^\mu \phi, \quad (4.78)$$

is invariant under the above $U(1)$ gauge transformation if we use the covariant derivatives

$$D_\mu \equiv \partial_\mu - ieA_\mu \quad (4.79)$$

¹¹In this book, it is simply called the Higgs mechanism.

with the vector field transforming as

$$A_\mu \longrightarrow A_\mu - \frac{i}{e} \partial_\mu \alpha(x). \quad (4.80)$$

Under the gauge transformation, the kinetic energy term $-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$ is also invariant. The potential which was originally U(1) invariant globally is still U(1) invariant locally since the potential does not involve spacetime derivatives. Thus, we can consider the potential shape given in Fig. 4.3. For the spontaneously broken case, i.e., with

$$\langle 0|\phi(x)|0\rangle = \frac{v}{\sqrt{2}}, \quad (4.81)$$

the U(1) gauge symmetry is broken. Now, let us study what is the mass spectrum of particles in this spontaneously broken *local* U(1) case. Firstly, the kinetic energy term of ϕ , evaluated in the unitary gauge

$$\phi = \frac{1}{\sqrt{2}} [v + \rho(x)] e^{ia(x)/v} \quad (4.82)$$

is

$$D_\mu \phi^* D^\mu \phi = \frac{1}{2} (\partial_\mu \rho)^2 + \frac{e^2}{2} (v^2 + 2v\rho + \rho^2) \left(A_\mu - \frac{1}{ev} \partial_\mu a \right)^2. \quad (4.83)$$

The potential becomes

$$V = \mu^2 \rho^2 + \lambda v \rho^3 + \frac{\lambda}{4} \rho^4 - \frac{1}{4} \mu^2 v^2. \quad (4.84)$$

Therefore, the radial field ρ obtains a mass

$$m_\rho^2 = 2\mu^2. \quad (4.85)$$

On the other hand, the phase field a does not have a mass term in (4.84). It looks like that it is a massless field. However, we have to be more careful here because of the original U(1) gauge symmetry. The kinetic energy term of a always appears as a combination of $(\partial_\mu a - evA_\mu)$ in (4.83), namely, a cannot be considered separately, but has to be considered with this combination, i.e., if we consider a new gauge field, we must consider the combination

$$A'_\mu = A_\mu - \frac{1}{ev} \partial_\mu a. \quad (4.86)$$

Then, a disappears completely from the total Lagrangian. The kinetic energy term of the gauge field is the same as before. The only change is that Eq. (4.83) contains

the $(A'_\mu)^2$ term of the form

$$\frac{1}{2}e^2v^2(A'_\mu)^2 + \dots,$$

which is interpreted as the mass term of the gauge boson A'_μ ,

$$M_A^2 = (ev)^2. \quad (4.87)$$

Is this a consistent picture? It is so. Originally, there were two real scalars (ρ, a) and a massless gauge field with two transverse components (for example in the radiation gauge $\vec{\nabla} \cdot \vec{A} = 0$). In the broken phase, there is one scalar ρ and one massive vector boson with three polarizations A'_μ (including the longitudinal component). Here, a becomes the longitudinal component of the gauge boson. So the number of the broken generators should match the number of massive gauge bosons after the spontaneous symmetry breaking. This phenomenon of rendering gauge bosons mass is the Higgs mechanism. In the Higgs mechanism, introduction of the scalar (fundamental or composite) field(s) is necessary to provide the longitudinal degrees of the massive gauge bosons. In this process, the radial field ρ acquires a larger mass $\sqrt{2}\mu$. This radial field is called the Higgs boson [12]. The mechanism leading to massive gauge bosons is called *spontaneous symmetry breaking* of gauge symmetries. But the existence of the fundamental Higgs boson is not a necessary condition to obtain a massive gauge field with spontaneous symmetry breaking. The spontaneous symmetry breaking just needs the property of the gauge symmetry breaking. The Higgs model with the fundamental scalars showed it explicitly with a bosonic Lagrangian. If the symmetry is spontaneously broken by the bilinear condensate of the fermion field, then it is not necessary to have the fundamental Higgs boson. But in this case, there appears a host of composite particles among which one [16] looks like the Higgs boson, but its property is quite different from the Higgs boson discovered at the LHC [17].

The proof we presented in this section for the loophole of the Goldstone theorem [14] is the mother of the Higgs mechanism. The method is applicable to any continuous symmetry. The idea of spontaneous symmetry breaking of any continuous symmetry is studied by the transformation of fields Ψ , under the continuous infinitesimal symmetry operation parameterized by ϵ ,

$$\delta_\epsilon \Psi = i\epsilon Q \Psi \quad (4.88)$$

where Q is some operator. Following the discussion of this section, the continuous symmetry is broken if $\langle \delta_\epsilon \Psi \rangle \neq 0$, which arises if there exists a state $|n\rangle$ which connects to $|0\rangle$ via nonvanishing components of $\langle 0|Q|n\rangle$. Then the state $|n\rangle$ is the Goldstone boson (Goldstone fermion, goldstino) if the symmetry parameter ϵ is a bosonic or commuting (fermionic or anti-commuting) degree.

Summarizing, as discussed in the boundary condition in the proof of the Goldstone theorem, the gauge theory does not necessarily imply a Goldstone boson

when the gauge symmetry is spontaneously broken since the gauge theory is not a manifestly covariant theory. We have seen explicitly that the relativistic QFT does not allow the Goldstone boson in the spontaneously broken gauge theory, but instead the corresponding gauge boson becomes massive. This phenomenon was discovered in 1963–64 by P. W. Higgs, F. Englert, R. Brout, G. S. Guralnik, C. R. Hagen, and T. W. B. Kibble. Though this mechanism was known in 1964, it was not applied to particle physics until 1967 when the SU(2) non-Abelian group for the charged current was used [18]. The argument toward the spontaneously broken gauge theory of weak interactions was made after the intermediate vector boson idea and the discovery of spontaneous symmetry breaking. In this series of developments, it looks like that “renormalizability” due to the absence of the gauge boson mass term played a significant role. Of course, it was not known then that the massless Yang–Mills theory is renormalizable, but it seems to be that a massless Yang–Mills theory looks better [18]. If the massless Yang–Mills theory is renormalizable, then the spontaneous symmetry breaking may not destroy the renormalizability, which was the argument in favor of spontaneously broken gauge theory to introduce massive gauge bosons. This idea led to the construction of the SM [19].

4.4.4. The ‘t Hooft mechanism

The so-called ‘t Hooft mechanism in gauge theories [20] is the following. Consider two continuous transformation parameters: one for a local transformation $\alpha(x)$ and the other for a global transformation β . They act on the field ϕ as

$$\phi \rightarrow e^{i\alpha(x)Q_{\text{gauge}}} e^{i\beta Q_{\text{global}}} \phi. \quad (4.89)$$

Basically, the $\alpha(x)$ direction becomes the longitudinal mode of massive gauge boson. It can be seen manifestly by redefining $\alpha(x)$ as $\alpha'(x) = \alpha(x) + \beta$,

$$\phi \rightarrow e^{i(\alpha(x)+\beta)Q_{\text{gauge}}} e^{i\beta(Q_{\text{global}}-Q_{\text{gauge}})} \phi, \quad (4.90)$$

$$\phi \rightarrow e^{i\alpha'(x)Q_{\text{gauge}}} e^{i\beta(Q_{\text{global}}-Q_{\text{gauge}})} \phi. \quad (4.91)$$

So, the charge $Q_{\text{global}} - Q_{\text{gauge}}$ is reinterpreted as the new global charge and is not broken by the VEV, $\langle \phi \rangle$. Basically, the direction β remains as the unbroken continuous direction. The ‘t Hooft mechanism is: *if a gauge symmetry and a global symmetry are broken by one VEV, then there remains a global symmetry*. It is used to derive an “invisible” axion from string theory, which will be discussed in Section 6.3.6.

4.5. Effects of quantum gravity

Quantum gravity effects break most symmetries except gauge symmetries [21]. Since there does not exist a universally accepted quantum gravity theory at present, our

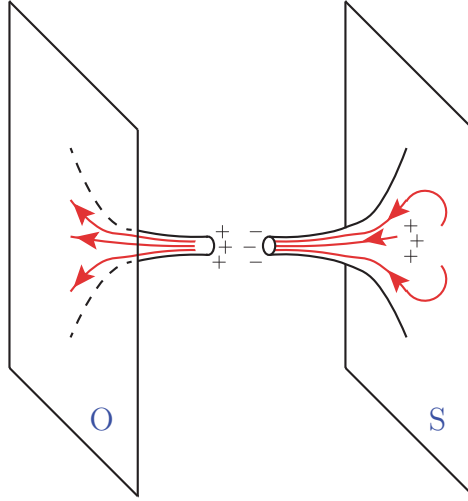


Fig. 4.4. A cartoon for a wormhole connecting the visible Universe and a shadow world. Figure taken from Ref. [22].

discussion may only proceed via classical aspects of the gravity sector by topology change, i.e., in connection with wormholes and black holes which can take information out of our visible Universe. In Fig. 4.4, a metric change of the observable world O to a shadow world S through a wormhole connection is depicted. If a $U(1)$ gauge charge, e.g., the electromagnetic charge e , is flown to the shadow world, it drags the flux lines. The effect to this metric change appears to the observer O as an effective interaction. The effective interaction in the visible Universe is obtained by cutting off the shadow world, i.e., by chopping off the neck of the wormhole. Then, one notices from Fig. 4.4 that the same amount of the flown-out charges are recovered to the observer O due to the presence of the $U(1)$ gauge flux lines.

However, if the flown-out charges are global charges, then there is no flux lines to drag and the observer O considers that he lost the global charges, namely, quantum gravity looks like violating global symmetries. This also applies to discrete symmetries which might be considered as a subgroup of some continuous group.

4.5.1. Discrete symmetries

Discrete symmetries are useful in two accounts. First, they limit possible interaction terms in the Lagrangian, which can simplify the study of cosmic evolution. Second, not all the possible discrete symmetries are ruled out from string theory and gravitational interactions. In gravity theory, some discrete symmetries are allowed while others are not. We can look into discrete symmetries from the bottom-up and top-down approaches.

Bottom-up

It can be easily understood from the fact that discrete symmetries can be a subgroup of some continuous symmetries. In low energy effective theory, discrete anomalies have been considered, and the safe discrete symmetries are called *discrete gauge symmetry* [23]. At field theory level with SUSY, there exists a host of literature on discrete symmetries [24–27]. In the bottom-up approach, it was discussed that $\mathbf{Z}_2$ symmetry is shown to be hairs [28].

Top-down

Low energy effective interactions from ultraviolet completed theories such as models from string compactifications can allow discrete symmetries [29, 30]. If discrete symmetries from string compactifications are considered, there is no worry about the gravity spoil of the resulting discrete symmetries because string compactifications admit anomaly-free gravity.

4.5.2. Global symmetries

Discrete symmetries in string compactification are the key ingredients in investigating effective low energy interactions. It became more important after realizing that gravity does not necessarily preserve global symmetries such as the Peccei–Quinn symmetry, which will be discussed more in Chapter 6.

In Fig. 4.5, we present a cartoon depicting the fate of global symmetries at low energy. The terms in the vertical (red and lavender) column are allowed by discrete symmetries from string compactification. If one considers a few leading effective terms, i.e., the terms corresponding to the lavender square, one can find an effective global symmetry. The global symmetry is respected by all terms in the horizontal (lavender and green) row. However, this global symmetry is broken by the terms in the red in the vertical column.

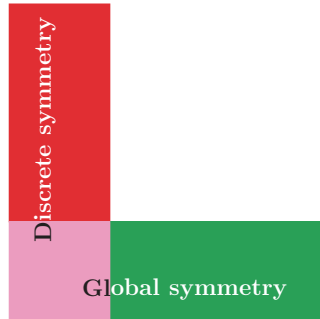


Fig. 4.5. A cartoon classifying symmetries at low energy. The terms in the vertical column are allowed by discrete symmetries in string compactification. If one considers a few leading effective terms, such terms define an effective global symmetry. However, this global symmetry is broken by the terms in the red.

4.6. Standard model

4.6.1. Convention on γ_5

The “V–A” theory prediction should not depend on the sign convention of γ_5 matrix. In the Bjorken–Drell notation, the “V–A” current is $\bar{\psi}\gamma^\mu(1 - \gamma_5)\psi$ while in the modern notation [4], the “V–A” current is $\bar{\psi}\gamma^\mu(1 + \gamma_5)\psi$. As in the above example, any convention is acceptable.

The “V–A” interaction for the neutron decay is

$$\mathcal{H} = \frac{G_F}{\sqrt{2}} \bar{e}\gamma_\mu(1 + \gamma_5)\nu_e \bar{p}\gamma_\mu(1 + \gamma_5)n + \text{h.c.} \quad (4.92)$$

The matrix element of the hadronic current of (4.92) between neutron momentum k and proton momentum k' is

$$\langle p(k') | \bar{p}\gamma^\mu(1 + \gamma_5)n | n(k) \rangle \equiv \bar{u}_p(k')\gamma^\mu(G_V(q^2) + G_A(q^2)\gamma_5)u_n(k) \quad (4.93)$$

$$\longrightarrow \bar{u}_p(k')\gamma^\mu(1 + g_A\gamma_5)u_n(k), \quad (4.94)$$

where the last line is in the $q^2 = 0$ limit with $q = k - k'$, and $G_V(q^2)$ and $G_A(q^2)$ are the vector and axial-vector form factors, respectively. The values at $q^2 = 0$ are the charges of the corresponding currents. Based on the conserved vector current (CVC) hypothesis, as in the case of conserved electromagnetic current, we take $G_V(0) = 1$. On the other hand, because of the *partially* conserved axial-vector current, $G_A(0) \equiv g_A$ is not 1, but determined at $\simeq 1.26$. Because strong interaction effects do not move the g_A direction depending on the sign convention of γ_5 , the cross-section should not involve an odd power of g_A , as expressed in Eqs. (2.54) and (2.56). One could have defined $g_A \simeq -1.26$, but we chose $g_A \simeq 1.26$. Physical processes are free of the sign convention on γ_5 .

4.6.2. Standard model

The current theory of modern particle physics is the SM based on the gauge group $\text{SU}(3)_c \times \text{SU}(2)_W \times \text{U}(1)_Y$, which is spontaneously broken as commented in the end of Section 4.4. One quark and lepton family is represented as¹²

$$\ell_e = \begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \quad e_R, \quad q_d^\alpha = \begin{pmatrix} u^\alpha \\ d^\alpha \end{pmatrix}_L, \quad u_R^\alpha, \quad d_R^\alpha, \quad (4.95)$$

$$Y: \quad \frac{-1}{2}, \quad -1, \quad \frac{+1}{6}, \quad \frac{+2}{3}, \quad \frac{-1}{3},$$

where $L = \frac{1+\gamma_5}{2}$ and $R = \frac{1-\gamma_5}{2}$ represent the left- and right-handed chiralities, respectively, and $\alpha = \{1, 2, 3\}$ is the color index. $\text{SU}(2)_W$ generators are T_i ($i = 1, 2, 3$) and $\text{U}(1)_Y$ generator is Y . In (4.95), the Y eigenvalues are also shown. The

¹²Sometimes, the R-handed e_R is represented by the L-handed e_L^c , which is convenient in GUTs.

number of two-component chiral fields in Eq. (4.95) is 15. It is said that there are 15 chiral fields in one family of the SM. For the BEHGHK mechanism, a complex Higgs doublet scalar H_d is introduced

$$H_d = \begin{pmatrix} H_d^0 \\ H_d^- \end{pmatrix}, \quad (4.96)$$

$$Y: \quad \frac{-1}{2}.$$

The Higgs mechanism discussed in Section 4.4 is achieved by the VEV of H_d ,

$$\langle H_d \rangle = \begin{pmatrix} \frac{v}{\sqrt{2}} \\ 0 \end{pmatrix}, \quad (4.97)$$

from which $W^\pm$, Z^0 , and photon obtain mass $\frac{1}{2}g_2v$, $\frac{1}{2}g_2|\cos\theta_W|$, and 0, respectively. The photon is not experiencing the Higgs mechanism because Q_{em} is realized in the Wigner–Weyl manner:

$$Q_{\text{em}}|0\rangle = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \frac{v}{\sqrt{2}} \\ 0 \end{pmatrix} = 0, \quad \text{where } Q_{\text{em}} = T_3 + Y. \quad (4.98)$$

It was observed by Kibble that spontaneous symmetry breaking of non-Abelian gauge symmetries can lead to a massless gauge boson by appropriately choosing an unbroken generator of the gauge group as in Eq. (4.98) [31]. This massless gauge boson is identified as photon in the SM.

At this point, it is worthwhile to comment on the electroweak scale $v \simeq 246 \text{ GeV}$ compared to the reduced Planck mass M_{P} or to the GUT-scale mass M_{GUT} . The problem to understand the small ratio, $v/M_{\text{P}} \sim 10^{-16}$, is the hierarchy problem. At present, there is no accepted solution to this hierarchy problem. The frontrunner among solutions of the hierarchy problem has been SUSY.

4.7. Weak CP violation

CP violation is the needed condition for baryogenesis starting from a $B = 0$ universe as discussed in Chapters 2 and 8. In the electroweak theory, the weak CP violation in the quark sector has been proved to be the Cabibbo–Kobayashi–Maskawa (CKM) model [32, 33]. In this model, three families of quarks are needed [33]. As shown in Fig. 4.6, three families of quarks and leptons, repeating representations (4.95) three times, introduce the flavor structure. Thus, at least 45 chiral fields are needed to describe weak CP violation. With three quark doublets, the CKM matrix is the phenomenological one for the weak interactions in the quark sector. With three lepton doublets, the Pontecorvo–Maki–Nakagawa–Sakata (PMNS) [34] matrix is the phenomenological one for the weak interactions in the lepton sector. These

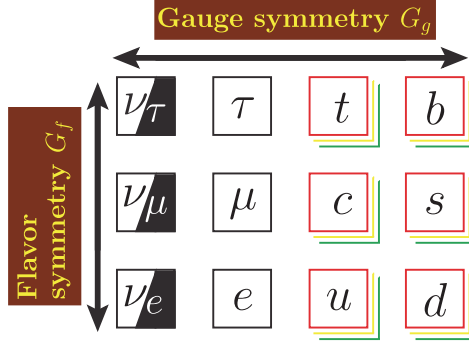


Fig. 4.6. Flavor space in the vertical direction. Only one chirality for neutrinos is implied by taking half squares.

matrices introduce parameters, δ_{CKM} and δ_{PMNS} , respectively, violating the discrete CP symmetry, in the quark and lepton sectors.

The well-known discrete symmetry in quantum mechanics is parity P. The Laporte rule, selecting P eigenstates in centrosymmetric molecules, was known even before the advent of quantum mechanics [35]. It was basically based on the P conservation in QED. This discrete symmetry P was later known to be broken outside QED, i.e., in weak interactions. In weak interactions, the discrete symmetry CP is also broken. To observe what will be the relation of the weak CP violation in gravity, we note that CP can be a discrete gauge symmetry in 10-dimensional supergravity [36]. Applying this to string compactification, the effective four-dimensional theories respect the CP symmetry. Then, the Yukawa couplings can be taken to be real. The weak CP violation at low energy must arise via the type of spontaneous CP violation [37] at a high energy scale. But, for the weak CP violation at the electroweak scale, it is enough to consider the Yukawa couplings generically complex, and the nature of spontaneous or hard breaking of CP at high energy scale is irrelevant.

Let us begin by presenting one way to count the number of physical parameters in the SM. For the representations (4.95), the family indices, $a = 1, 2, 3$, are attached. The u - and d -type quark mass matrices are denoted by $M^{(u)}$ and $M^{(d)}$, respectively, and e - and ν -type lepton mass matrices by $M^{(e)}$ and $M^{(\nu)}$, respectively. Let us start with diagonalized mass matrices, $M^{(d)}$ and $M^{(e)}$, with real eigenvalues, $m_d, m_s, m_b, m_e, m_\mu$, and m_τ . For the Higgs doublet of (4.97), we can take VEV as a real one. As commented above, the Yukawa couplings of u quarks to $H_u = i\sigma_2 H_d^*$ are taken to be complex. Now, we diagonalize $M^{(u)}$ by bi-unitary transformation with two independent unitary matrices U^L and U^R ,

$$M^{(u),\text{diag}} = U^{L\dagger} M^{(u)} U^R. \quad (4.99)$$

With completely general complex Yukawa couplings of H_u , $M^{(u)}$ has 18 real parameters. Two unitary matrices, U^L and U^R , have 18 parameters. But, we will not consider the overall phase of U^L and U^R , as commented below as the baryon number.

The total number of parameters we introduced except the baryon number is 34. The Yukawa couplings are of the form $f_{ab}^{(u)} \bar{u}_L^a u_R^b H_u$ which conserve the quark number or baryon number B . The neutral gauge interactions are flavor-diagonal and hence real. The charged current interactions are

$$\frac{g}{\sqrt{2}} \sum_a \bar{u}_L^a \gamma^\mu d_L^a W_\mu^+ = \frac{g}{\sqrt{2}} \bar{u}_L^{\text{diag}} \gamma^\mu V_{\text{CKM}} d_L^{\text{diag}} W_\mu^+, \quad (4.100)$$

which also conserve the baryon number. With the bi-unitary transformation on the L-handed fields, $u_L^a = U_{ab}^L u_L^{b,\text{diag}}$, we identify the CKM matrix as $V_{\text{CKM}} = U^L$. Now, there is a freedom of redefining phases of $u_L^{a,\text{diag}}$ and $u_R^{a,\text{diag}}$ fields, whose total number is six. These may be used to remove parameters. But the overall phase, corresponding to the B number, cannot be used for this purpose, since the overall phase corresponding to B does not appear in Eq. (4.100) and also in $\bar{u}_L^{a,\text{diag}} M^{(u),\text{diag}} u_R^{a,\text{diag}}$. Therefore, only five phases can be removed. Now, let us count the independent parameters. Not considering the overall phases from U^L and U^R , only 34 parameters are considered from U^L and U^R . The conditions in Eq. (4.99) are 18. At this point, note that the total number of constraints are 23 ($= 5 + 18$). Thus, there remain 11 parameters out of 34, which are m_u, m_c, m_t and two determinants $= 1$ matrices U^L and U^R . U^L and U^R must have the same number of parameters, each with 4, because the same physics is described by the exchange of L and R . Thus, the determinant $= 1$ unitary matrix $U^L = V_{\text{CKM}}$ has four parameters. Since a general 3×3 orthogonal matrix has three real parameters, the unremovable CP phase for three families of quarks is one [33]. Let us represent this CP phase as δ_{CKM} .

Now, it is convenient to express the four parameter charged currents as the CKM matrix [38],

$$\begin{pmatrix} c_1, & s_1 c_3, & s_1 s_3 \\ -c_2 s_1, & e^{-i\delta_{\text{CKM}}} s_2 s_3 + c_1 c_2 c_3, & -e^{-i\delta_{\text{CKM}}} s_2 c_3 + c_1 c_2 s_3 \\ -e^{i\delta_{\text{CKM}}} s_1 s_2, & -c_2 s_3 + c_1 s_2 c_3 e^{i\delta_{\text{CKM}}}, & c_2 c_3 + c_1 s_2 s_3 e^{i\delta_{\text{CKM}}} \end{pmatrix}, \quad (4.101)$$

where $c_i = \cos \theta_i$ and $s_i = \sin \theta_i$ for $i = 1, 2, 3$. In this form, the invariant quantity for the CP violation, the so-called the Jarlskog determinant [39], is $J = |\text{Im } V_{13} V_{22} V_{31}| \simeq \mathcal{O}(\lambda^6)$ [40] where $\lambda \simeq 0.22$ is the Cabibbo parameter $\lambda = \sin \theta_C$ [32]. Because $e^{i\delta_{\text{CKM}}}$ in the (31) element is an overall phase, i.e., $V_{\text{CKM}(31)} = -|V_{\text{CKM}(31)}| e^{i\delta_{\text{CKM}}}$, it directly gives the information on δ_{CKM} because $|V_{\text{CKM}(31)}| = \mathcal{O}(\lambda^3)$ and $|V_{\text{CKM}(13)}| = \mathcal{O}(\lambda^3)$, and $J = \mathcal{O}(\lambda^6)$. The Feynman diagram, Fig. 4.7 (a), has the charged current coupling with parameters of $V_{\text{CKM}} = V$. The up-type quark mass term is shown in Fig. 4.8(a).

In the lepton sector, we adopt the majority view that the light fermions in the SM are only 15 chiral fields of Eq. (4.130). Then, neutrino masses are only of the Majorana type. Now, we can define a similar kind of charged current interactions between mass eigenstates as shown in Fig. 4.7(b) where U is the so-called PMNS

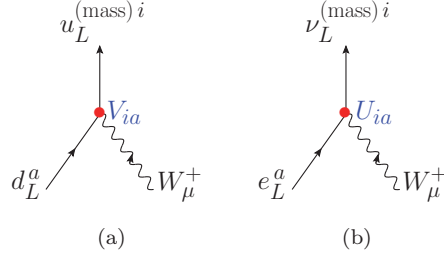


Fig. 4.7. Charged current interactions with mass eigenstates: (a) in the quark sector, and (b) in the lepton sector. Here, $M^{(d)}$ and $M^{(e)}$ are already diagonalized.

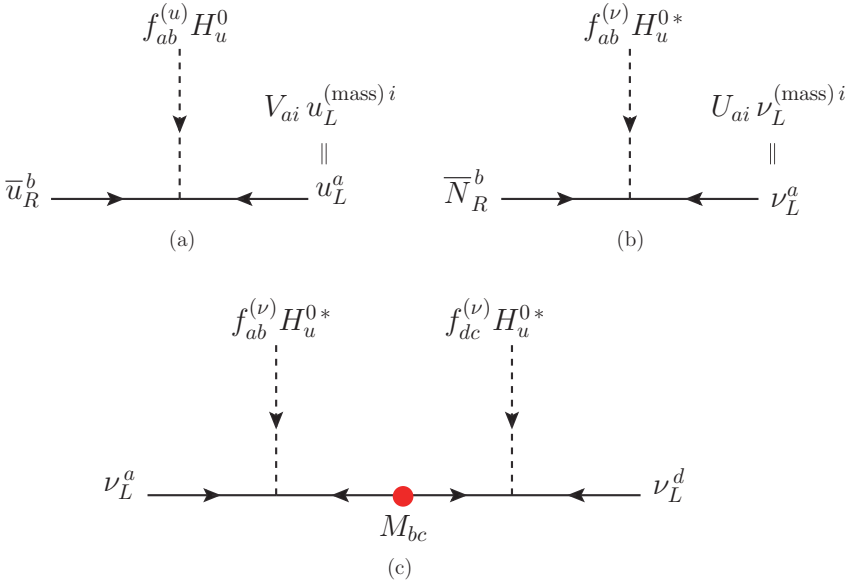


Fig. 4.8. The u -type quark and neutral lepton mass terms: (a) Dirac masses of u -type quarks, (b) Dirac masses of neutral leptons, and (c) Majorana masses of ν . The Majorana masses of heavy neutrinos N are not shown.

matrix [34], $U_{\text{PMNS}} = U$ which is used for converting the mass eigenstates of neutrinos to the weak eigenstates of neutrinos, $\nu_L^a = U_{ab} \nu_L^{b, \text{diag}}$. In Fig. 4.7(b), charged leptons are assumed to be already diagonalized.

As shown in Fig. 4.8(c), the neutrino mass term is symmetric, $\frac{1}{2} \nu^T M^{(\nu)} \nu$, violating the lepton number by two units, where $M^{(\nu)}$ is complex and symmetric. A complex symmetric matrix A can be “diagonalized” using one unitary matrix U , where $U^T A U$ is a real diagonal matrix, which is called the Autonne–Takagi factorization [41],

$$M_{\alpha\beta}^{(\nu) \text{diag}} = U_{i\alpha} M_{ij}^{(\nu)} U_{j\beta}, \quad (4.102)$$

which is not a unitary transformation. Multiplying ν^{diag} on both sides, we obtain

$$\nu^{\text{diag},\alpha} M_{\alpha\beta}^{(\nu)\text{diag}} \nu^{\text{diag},\beta} = \nu^{\text{diag},\alpha} U_{i\alpha} M_{ij}^{(\nu)} U_{j\beta} \nu^{\text{diag},\beta}. \quad (4.103)$$

Unlike in the quark case, there is no lepton number conservation, i.e., we do not have a freedom to phase-rotate the neutrino fields in the diagonalizing condition (4.102). Note that both left- and right-hand sides of (4.103) break the lepton number by the same unit. The total number of conditions we impose in (4.102) is 18. The total number of parameters we introduced was 27: 18 from $M^{(\nu)}$ and 9 from U . Imposing 18 conditions of (4.102), there remain nine physical parameters. These are three neutrino masses, two Majorana phases, and $\Theta_1, \Theta_2, \Theta_3$, and δ_{PMNS} . Since the PMNS matrix can appear in the type-II leptogenesis as discussed in Chapter 8, the following PMNS matrix U_{PMNS} is useful, viz. Fig. 4.8(b):

$$\begin{pmatrix} C_1, & S_1 C_3, & S_1 S_3 \\ -C_2 S_1, & e^{-i\delta_{\text{PMNS}}} S_2 S_3 + C_1 C_2 C_3, & -e^{-i\delta_{\text{PMNS}}} S_2 C_3 + C_1 C_2 S_3 \\ -e^{i\delta_{\text{PMNS}}} S_1 S_2, & -C_2 S_3 + C_1 S_2 C_3 e^{i\delta_{\text{PMNS}}}, & C_2 C_3 + C_1 S_2 S_3 e^{i\delta_{\text{PMNS}}} \end{pmatrix},$$

where $C_i = \cos \Theta_i$ and $S_i = \sin \Theta_i$ for $i = 1, 2, 3$. Possibilities of relating δ_{CKM} and δ_{PMNS} and δ_{PMNS} and leptogenesis phases have been discussed in [42] and in Chapter 8, respectively.

We stress that physical processes depending on these phases must be parameterization-independent, for example, the Jarlskog invariant in the case of CP violation in hadron physics must be the same whichever parameterization one uses. The Jarlskog invariant is given by $J = |\text{Im } V_{13} V_{22} V_{31}| \simeq \mathcal{O}(\lambda^6)$ [40] for the CKM matrix (4.101), which shows that all three families must participate to have a nonzero J . Observation of CP violation is based on the interference phenomenon, involving all three families.

4.8. Global SUSY

SUSY is probably the most amazing symmetry ever since the discovery of isospin. It can be introduced in many different ways. It is a symmetry unifying fermions and bosons, and the space it is acted on is called *superspace* [43]. The supercharge Q is the generator for the SUSY transformation of fermions to bosons and vice versa:

$$Q|F\rangle = |B\rangle, \quad Q|B\rangle = |F\rangle. \quad (4.104)$$

From the definition of supercharge in (4.104), we note that Q must be spinorial because both $Q|B\rangle$ and $|F\rangle$ must transform like a spinor under rotation. The spinorial charge Q has two components, and we use in most cases the Weyl spinors in SUSY [8]. A left-handed (L-handed) Weyl fermion can be obtained from a complex scalar by operating Q . So, Q transforms like a left-handed Weyl fermion. A right-handed (R-handed) fermion and the corresponding complex scalar can be

said similarly. This is the reason that we can define the chirality of scalars in SUSY. The scalar chirality can be helpful to obtain light scalars. If we succeed in this F and B unification, that alone can be a merit.

The Lorentz algebra $SO(3,1)$ is the same as $SU(2) \times SU(2)$, and the Lorentz group $SO(3,1)$ can be locally viewed as $SU(2) \times SU(2)$. The Weyl fermion transforms as $(\mathbf{2}, \mathbf{1})$ or as $(\mathbf{1}, \mathbf{2})$ under $SU(2) \times SU(2)$. Let $(\mathbf{2}, \mathbf{1})$ be the L-handed field and $(\mathbf{1}, \mathbf{2})$ be the R-handed field. The indices for $SU(2)_L$ are denoted as undotted $\alpha = \{1, 2\}$ and the indices for $SU(2)_R$ are named as dotted $\dot{\alpha} = \{\dot{1}, \dot{2}\}$ [8]. Since Q transforms like a L-handed Weyl spinor, its commutation relation with the angular momentum generator $J^{\mu\nu}$ is

$$[J^{\mu\nu}, Q_\alpha] = -i(\sigma^{\mu\nu})_\alpha^\beta Q_\beta. \quad (4.105)$$

For the R-handed Weyl fermions and their accompanying complex scalars, the supercharge must transform nontrivially under $SU(2)_R$. Let us call this supercharge $\overline{Q}$ which changes the dotted indices,

$$[J^{\mu\nu}, \overline{Q}_{\dot{\alpha}}] = -i(\overline{\sigma}^{\mu\nu})_{\dot{\alpha}}^{\dot{\beta}} \overline{Q}_{\dot{\beta}}. \quad (4.106)$$

$\overline{Q}$ is the charge conjugated of Q , since L changes to R and vice versa under charge conjugation. The total number of complex components in Q and $\overline{Q}$ is four. Thus, we can form the following representation for the supercharge in the Weyl representation:

$$\mathcal{Q} = \begin{pmatrix} Q \\ \overline{Q} \end{pmatrix}. \quad (4.107)$$

There exists the famous no-go theorem by Coleman and Mandula [44] which says that the fermion–boson symmetry and the spacetime symmetry cannot be unified in a naïve way, just by making the internal space bigger, i.e., making the Lie group bigger. SUSY escapes this Coleman-Mandula theorem by not making just the Lie group bigger, but by introducing an algebra outside the Lie algebra. It is called the graded Lie algebra where one adds anticommutators for some generators. With four supercharges, i.e., corresponding to $\mathcal{Q}$ of Eq. (4.107), we have the $\mathcal{N}=1$ SUSY algebra,

$$\{Q_\alpha, \overline{Q}_{\dot{\beta}}\} = 2(\sigma^\mu)_{\alpha\dot{\beta}} P_\mu, \quad (4.108)$$

$$\{Q_\alpha, Q_\beta\} = 0, \quad \{\overline{Q}_{\dot{\alpha}}, \overline{Q}_{\dot{\beta}}\} = 0. \quad (4.109)$$

With the space translation generators P_μ , we have the following commutation relations:

$$[P_\mu, Q_\alpha] = 0, \quad [P_\mu, \overline{Q}_{\dot{\alpha}}] = 0, \quad [P_\mu, P_\nu] = 0. \quad (4.110)$$

The parameter for the SUSY transformation, ϵ , must transform like a spinor under rotation so that $\overline{Q}\epsilon$ transforms like a scalar. SUSY was introduced in 1971 [45], but

the linear realization (4.104) of SUSY, what we use today, is due to the work of Wess and Zumino [46].

The time component of the algebra (4.108) gives the Hamiltonian in terms of supercharges

$$H = P^0 = \frac{1}{4}(Q_1\bar{Q}_1 + \bar{Q}_1Q_1 + Q_2\bar{Q}_2 + \bar{Q}_2Q_2), \quad (4.111)$$

which implies that the energy eigenvalues are nonnegative. We consider only $\mathcal{N}=1$ SUSY where the introduction of chirality is possible.

If SUSY is unbroken, i.e., realized in the Wigner–Weyl manner, the supercharges annihilate the vacuum $|0\rangle$, and the vacuum energy is zero,

$$\text{Global SUSY: } E_{\text{vac}} \geq 0, \text{ equality for the unbroken SUSY.} \quad (4.112)$$

Although we do not use the superfield formalism [43] here, we list its powerful constraints on the form of Lagrangian. Introducing an anticommuting coordinate ϑ^α ($\alpha = 1, 2$) and $\bar{\vartheta}_{\dot{\alpha}}$ ($\dot{\alpha} = \dot{1}, \dot{2}$), one can also introduce a quantum field as a function of x, ϑ and $\bar{\vartheta}$ [8]. A polynomial of ϑ includes only three terms, 1, ϑ , and ϑ^2 , and similarly for $\bar{\vartheta}$. In view of the $\text{SU}(2)_L \times \text{SU}(2)_R$ property of the Lorentz group (viz. Eqs. (4.105), (4.106)), $\vartheta(\bar{\vartheta})$ is a doublet under $\text{SU}(2)_L$ ($\text{SU}(2)_R$) of the Lorentz group. For fermions, we introduce an L-handed chiral field ψ , which is a singlet under $\text{SU}(2)_R$. This ψ can make a singlet of $\text{SU}(2)_L$ (viz. $\mathbf{2} \times \mathbf{2} = \mathbf{1} + \mathbf{3}$), by taking the antisymmetric combination with ϑ , $\vartheta\psi \equiv \epsilon_{\alpha\beta}\vartheta^\alpha\psi^\beta$ where $\epsilon_{\alpha\beta}$ is the Levi-Civita tensor of $\text{SU}(2)_L$. Thus, $\text{SU}(2)_L$ singlets can be a scalar function of $\varphi(x)$ and $\psi(x)\psi(x)$, which is denoted as ϕ , a function of the forms $\vartheta\psi(x)$ and $F(x)\vartheta\vartheta$.

4.8.1. Chiral field

A (L-handed) chiral superfield $\Phi(x, \vartheta)$ is defined as a function of ϑ only, thus a *chiral superfield* has an expansion¹³

$$\Phi(x, \vartheta) = \phi(x) + \vartheta^\alpha\psi_\alpha + \vartheta^\alpha\vartheta^\beta\epsilon_{\alpha\beta}F(x). \quad (4.113)$$

The chiral superfield Φ contains a spin-0 boson and a spin- $\frac{1}{2}$ fermion, as implied in Eq. (4.104). The scalar field is $\phi(x)$ and the fermion field is $\psi(x)$. The so-called auxiliary field $F(x)$ is the coefficient of $\vartheta\vartheta$ in Eq. (4.113).

4.8.2. Vector field

A superfield containing both ϑ and $\bar{\vartheta}$ has more degrees. Here, it is possible to introduce a spin-1 boson in the superfield $\mathcal{V}$, with the reality condition $\mathcal{V} = \mathcal{V}^\dagger$. $\mathcal{V}(x, \vartheta, \bar{\vartheta})$ is called a vector superfield.

¹³Similarly, from the consideration of $\text{SU}(2)_R$, an R-handed chiral field $\Phi^\dagger(\bar{z})$ can be given.

F and D terms

The action in the superspace is $\int d^4x$ times

$$\int d^2\vartheta W(\vartheta) = \int d^2\vartheta F_W(\Phi), \quad (4.114)$$

$$\int d^2\vartheta \int d^2\bar{\vartheta} K(\Phi, \Phi^*), \quad (4.115)$$

where the first term is picking up the F term of the superpotential W and the second is picking up the D term of the Kähler potential K . The integral with the anticommuting ϑ and $\bar{\vartheta}$ is equivalent to differentiating with respect to ϑ and $\bar{\vartheta}$. Thus, from a function of superfields, we pick up the last term, i.e., the F component of $W(\phi) = A_W + \psi_W\vartheta + F_W\vartheta^2$. The integration with $\int d^2\vartheta$ removes ϑ^0 and ϑ^1 terms, and for the ϑ^2 term drops only ϑ^2 . Similarly, the D term of K is picked up by $\int d^2\vartheta \int d^2\bar{\vartheta}$.

4.8.3. *R symmetry*

The chiral parameter ϑ is complex, which can be written with a phase. A phase shift of ϑ is called $U(1)_R$ transformation, which is the R symmetry

$$R: \begin{cases} \vartheta \rightarrow e^{-i\alpha}\vartheta, \\ W(\phi) \rightarrow e^{2i\alpha}W(\phi), \end{cases} \quad (4.116)$$

i.e., the superpotential $W(\phi)$ must have two units of R -charge such that the R symmetry can be defined.

This superfield formalism is quite useful in analyzing the form of the allowed action. Firstly, note that the globally supersymmetric Lagrangian depends only on three functions K, W , and the gauge kinetic function f [8]:

- Kähler potential $K(\{\phi_i\}, \{\phi_i^*\})$ for $i = 1, 2, \dots$, a Hermitian function, determines mainly the kinetic terms of chiral multiplets.
- Superpotential $W(\{\phi_i\})$ for $i = 1, 2, \dots$, a holomorphic function, i.e., a function of the L-handed chiral scalars ϕ_i only, determines the potential $V(\{\phi_i\}, \{\phi_i^*\})$. Similar comments apply to the R-handed chiral scalars with $\overline{W}(\{\phi_i^*\})$.
- Gauge kinetic function $f_{ab}(\{\phi_i\})$, a holomorphic function, is the coefficient of gauge kinetic terms.

In particular, the scalar potential is always positive definite

$$V(\phi, \phi^*) = \sum_i \left| \frac{\partial W(\phi)}{\partial \phi_i} \right|^2 + \frac{1}{2} f_{ab} D^a D^b, \quad (4.117)$$

where we replaced the superfield Φ with its scalar component ϕ and $D^a = G^i T_i^{aj} \phi_j$ is the D term. There is the *nonrenormalization theorem*: Because of the holomorphicity, the superpotential $W(\Phi)$ does not receive loop corrections other than those of wave function renormalization, at all orders of perturbation theory. Also, the gauge kinetic function $f_{ab}(\Phi)$ does not receive higher order corrections beyond one loop order. These are quite restrictive compared to nonsupersymmetric models.

4.9. Supergravity

In this section, we introduce some interaction formulas in supergravity which are needed in this book. In supergravity, the SUSY transformation parameter ϵ is promoted to be local, i.e., it is dependent on x_μ . If SUSY is the symmetry of the action, it must be severely broken since the superpartner of the electron has not been discovered up to 2 TeV. If the global SUSY is broken at the scale M_S , the vacuum energy must be of the order M_S^4 , in view of (4.112). The extremely small vacuum energy excludes the global SUSY. This is the phenomenological reason to extend the global SUSY to the local one.

A better reason may be to include gravity within the SUSY framework. The local SUSY is also called *supergravity*. If the vacuum energy problem is not resolved in supergravity as well, then this would be just an academic exercise. Fortunately, supergravity allows the possibility of introducing a zero cosmological constant after SUSY breaking [47]. But the vanishing cosmological constant is achieved by fine-tuning parameters in the SUSY Lagrangian.

In the supergravity Lagrangian, K and W appear within a single functional form G ,

$$G(\phi, \phi^*) = -3 \log(-K/3) + \log |W|^2, \quad (4.118)$$

where we set the reduced Planck mass $M_P = 1$. This oddly looking coefficients without dimensions are for the convenience of notation. The function (4.118) has a symmetry

$$\begin{aligned} 3 \log(-K/3) &\rightarrow 3 \log(-K/3) + h(\phi) + h^*(\phi^*), \\ W &\rightarrow e^{-h} W. \end{aligned} \quad (4.119)$$

Covariant and contravariant indices are used for holomorphic and antiholomorphic scalars, respectively. The Kähler metric of the (sigma model) target space is defined as

$$G^i = \frac{\partial G}{\partial \phi_i}, \quad G_i = \frac{\partial G}{\partial \phi^{*i}}, \quad G_j^i = \frac{\partial^2 G}{\partial \phi_i \partial \phi^{*j}}. \quad (4.120)$$

Then, the bosonic Lagrangian is given by

$$e^{-1}\mathcal{L} = \frac{\mathcal{L}}{\sqrt{g}} = -\frac{1}{2}R + G^i{}_j D_\mu \phi_i D^\mu \phi^{*j} + \frac{1}{4}\text{Re}(f_{ab})F_{\mu\nu}^a F^{b\mu\nu} + \frac{1}{8}\text{Im}(f_{ab})\epsilon^{\mu\nu\rho\sigma} F_{\mu\nu}^a F_{\rho\sigma}^b + V(\phi, \phi^*) \quad (4.121)$$

with the following scalar potential [48, 49]:

$$V(\phi, \phi^*) = e^K [(G^{-1})^i{}_j D_i W^* D^j W - 3|W|^2] + \frac{1}{2}f_{ab}D^a D^b, \quad (4.122)$$

where

$$D^i W = \frac{\partial W}{\partial \phi_i} + \frac{\partial K}{\partial \phi_i} W, \quad D_i W^* = \frac{\partial W^*}{\partial \phi^{*i}} + \frac{\partial K}{\partial \phi^{*i}} W^*, \quad (4.123)$$

and

$$D^a = G^i T_i^{aj} \phi_j, \quad (4.124)$$

which is the on-shell D term. In contrast to the global SUSY case (4.117), here the superpotential is not positive definite, viz. the $-3|W|^2$ term in (4.122).

The SUSY breaking condition can be read from the transformation laws of fermionic fields. For SUSY breaking, only their scalar components can assume VEVs that do not violate the Lorentz symmetry,

$$\delta_\epsilon \Psi \sim -e^{G/2} \frac{1}{W^*} D_i W^* \epsilon - \frac{1}{8} \frac{\partial f_{ab}}{\partial \phi^{*j}} \lambda_a \lambda_b \epsilon, \quad (4.125)$$

$$\delta_\epsilon \lambda \sim \frac{i}{2} g \text{Re} f_{ab}^{-1} G^i (T_b)_i^j \phi_j \epsilon. \quad (4.126)$$

The right-hand side of (4.125) is called the F term of Ψ . SUSY can be broken if the F term is nonvanishing, either by (i) the first term assuming VEV or (ii) the second term through the gaugino (λ_a) condensation by some strong force. The SUSY breaking scale for case (i) is

$$M_S^2 = e^{G/2} \frac{1}{W^*} D_i W^*, \quad (4.127)$$

and a similar expression holds for case (ii).

Supergravity formulated with an AdS curvature $\overline{\Lambda} < 0$ has a negative vacuum energy $\overline{\Lambda}$. With broken SUSY, a positive constant (viz. (4.112) and (4.122)) is added to $\overline{\Lambda}$, making it possible for the vacuum energy in the broken phase to be zero, $V_0 = 0$. For example, if SUSY is broken by the nonzero F term only, then the flat space condition requires $G_{0k} G_0^k = 3$. In this flat limit, the gravitino mass is

$$m_{3/2} = M_P e^{G_0/2}, \quad (4.128)$$

where M_P is the reduced Planck mass, 2.44×10^{18} GeV. Thus, supergravity saves us from the disaster of a huge cosmological constant. But, it must be remembered

that we achieved the flat space by a fine-tuning, since the initial curvature $\bar{\Lambda}$, with which we formulated the theory, is an arbitrary number. In addition, if gravitino obtains a large mass, the R symmetry of (4.116) is badly broken.

We introduce the interactions of matter by their Yukawa couplings. The R-handed fields can be considered to be the charge conjugated L-handed fields. The lowest order Yukawa couplings¹⁴ are obtained from the cubic terms of the superpotential W . In W , fields are denoted by the first components of chiral fields, i.e., by scalar components. The scalar partners of fermions are called sfermions, e.g., squark, selectron, and sneutrino. On the other hand, the fermionic partners of bosons carry the suffix “ino”, e.g., higgsinos, gauginos, gravitinos, etc. Supersymmetrization of Higgs bosons require the higgsinos to be L-handed so that they can couple with other L-handed fields in W . As noted before, scalars in supersymmetric theory have chiralities which are determined by the chirality of their fermionic partner.

4.9.1. Minimal SUSY standard model

If we consider gauge bosons, their fermionic partners ($s = \frac{1}{2}$) are called gauginos, e.g., gluino, wino, zino, photino, and bino. Here, bino means the partner of the $U(1)_Y$ gauge boson B_μ . To give mass to an electron, we can consider a superpotential, $l_L e_L^c H_d$. Down-type quarks can obtain mass by the term, $q_L d_L^c H_d$ in Eq. (4.95), however up-type quarks cannot obtain mass by H_d . They need the $Y = +\frac{1}{2}$ higgsino doublet H_u . Unlike the case without SUSY, $i\sigma_2 H_d^*$ cannot serve for the up-type quark mass since the charge conjugated field is R-handed and W does not allow couplings of both chiralities. Therefore, we need another L-handed Higgs doublet H_u for the up-type quark masses, $q_L u_L^c H_u$. It is also needed to cancel the gauge anomaly since we considered the complex fermion through supersymmetrization of H_d . The addition of H_u makes the representation $H_d \oplus H_u$ real under $SU(3) \times SU(2) \times U(1)$. The $\mathcal{N}=1$ SUSY model with three families and one set of H_u and H_d is called the minimal supersymmetric standard model (MSSM). The MSSM consists of three families, e family, μ family, τ family, and the pair of Higgs doublets. The chiral fields of the MSSM are

$$\text{MSSM} : e \text{ family} \oplus \mu \text{ family} \oplus \tau \text{ family} \oplus H_d \oplus H_u. \quad (4.129)$$

Here, one family contains 15 chiral fields, for example, for the e family, they are

$$l_L \equiv \begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \quad e_L^c, \quad q_L \equiv \begin{pmatrix} u \\ d \end{pmatrix}_L, \quad u_L^c, \quad d_L^c. \quad (4.130)$$

The MSSM has a problem of why the term $\mu H_u H_d$ is forbidden in the superpotential. The R symmetry, Eq. (4.116), may be used, but it is broken in supergravity since gravitino must be massive. The μ problem can be solved by spontaneously

¹⁴More generally, the couplings between two fermions and many scalars can be called Yukawa couplings.

broken Peccei–Quinn symmetry at the intermediate scale [50], which is the Kim–Nilles mechanism [51].

4.9.2. *SUSY GUTs*

This leads us to the obvious unification, the supersymmetrized GUTs or SUSY GUTs. GUTs are theories unifying the weak, electromagnetic, and strong interactions with a single gauge coupling constant. This can be achieved with a simple group [52, 53] or with a semi-simple group (supplemented by some additional discrete symmetries to identify the gauge coupling constants) [54].

The MSSM can be easily extended to SUSY GUTs [55], with 15 chiral fields of Eq. (4.130) assembled in $\mathbf{10}$ and $\bar{\mathbf{5}}$ (repeated three times), and H_u and H_d (only once) in $\mathbf{5}$ and $\bar{\mathbf{5}}$, of $SU(5)$. To break SUSY GUTs into the MSSM, one used the adjoint matter field before [55]. In string compactification, antisymmetric tensor fields are more useful for breaking the GUT group than the adjoint representation. These $SU(N)_{\text{anti}}$ GUTs were proposed before [56] and $SU(7)_{\text{anti}}$ has been constructed for a family-unified GUT from string theory [57]. The $SU(5)_{\text{anti}}$ is basically $SU(5)_{\text{flip}} \equiv SU(5) \times U(1)$ [58].

4.9.3. *From ultraviolet completed theories*

Ultraviolet completed theories in the theme of unification have been proposed to include gravity [59] and to understand the light $H_u \oplus H_d$ doublets in extra dimensions [60].

To understand just the hierarchy between M_P and v_{ew} , extra dimensions have also been considered [61]. More interesting consideration of extra dimensions was to introduce the warp factors [62, 63]. Reference [59] is string theory and Refs. [60–63] are QFT models.

Among these, only string theory includes gravity, and compactification of string theory is the key toward obtaining the MSSM.

4.10. Summary of elementary particle DM

Particle candidates for CDM must have survived until now, with their lifetime greater than the age of the Universe $t_U \simeq 4.3 \times 10^{17} \text{ s} \simeq 0.16 \cdot 10^{-42} \text{ GeV}^{-1}$. If the hypothetical particle X decays by the following interaction:

$$\frac{1}{M^n} \phi_1 \cdots \phi_\ell X, \quad (4.131)$$

where ϕ 's are bosons or fermions, then an eyeball decay width of X to massless ϕ 's is

$$\Gamma \approx \frac{M_X^{2n+1}}{\tilde{M}^{2n}} (\text{phase space factor}) = (\text{phase space factor}) \left(\frac{M_X}{\tilde{M}} \right)^{2n} M_X. \quad (4.132)$$

For axion, we can take $n = 1$, $\tilde{M} \sim 10^{13}$ GeV, $M_X = 10^{-5}$ eV, and phase space factor $\sim 10^{-2}$, and thus obtain $\Gamma \approx 10^{-61}$ eV $\approx 1/10^{41}$ years $\ll 1/t_U$. For $n = 1$, a keV particle needs $\tilde{M} > 2.5 \times 10^{11}$ GeV for it to live longer than the age of the Universe. Masses and interaction strengths give various possibilities, some of which we list below. All these particle candidates are based on the symmetry principles we discussed in this chapter, namely, the bosonic coherent motions with *spontaneously broken* global symmetries or unbroken (exact or almost exact) conserved charges. The bosonic coherent motion and the conserved charge scenarios will be discussed in more detail in Chapters 6 and 7, respectively. The first two candidates in the following interact via the SM interactions.

- **Minimal dark matter:** Minimal DM arises in the case of introducing higher dimensional representation such as the representation **5** under $SU(2)_W$ such that there is no gauge anomaly. It is named minimal because no new interaction is introduced except one higher dimensional representation [64].
- **Right-handed neutrinos:** The right-handed neutrino is the case by introducing R-handed doublets.
- **Mirror DM:** Mirror DM is the case where the model has the $L \leftrightarrow R$ symmetry, where higher decoupling temperature for the mirror world is possible [65].
- **Axion:** The box on axion in Fig. 1.4 is for the very light QCD axion. The “invisible” axion solves the strong CP problem, which is a kind of hierarchy problem. It will be discussed in more detail in Chapter 6.
- **WIMP:** The box marked “WIMP” in Fig. 1.4 represents “generic” weakly interacting massive particle candidates produced in the Universe as *thermal relics*. Their mass can lie in the range between a few GeV (below which it would overclose the Universe) and some ~ 100 TeV. The most highly scrutinized thermal relic is the lightest neutralino particle in SUSY theories, hereafter referred to as simply the neutralino. The neutralino is particularly well motivated since, in addition to solving the DM problem, SUSY extensions of the SM contain a number of other attractive features both on the particle physics side and in the early Universe cosmology. In addition to the neutralino, there are a host of WIMPs suggested in the literature. These have the weak-scale scattering cross-sections with their masses to lie above a few GeV to the ~ 1 TeV scale, based on some suggested theoretical expectation. These will be discussed in more detail in Chapter 7.
- **E-WIMP:** The extra- or extraordinarily-weakly interacting particle is E-WIMP. Axinos can be either thermal or nonthermal relics, or both, since they can be produced in both thermal production and nonthermal processes. Sometimes, the phrase “feebly interacting massive particle” is used for this category. The best known particle in this category is *axino* which is the superpartner of axion [66]. Axino can be hot, warm, or cold, which will be discussed in more detail in Chapter 7.

- **Gravitino:** With SUSY, supergravity theory predicts the *gravitino* $\tilde{G}$, the fermionic partner of the graviton. It is another well-motivated example of an E-WIMP. Gravitino can be hot, warm, or cold, as distinguished by colors in Fig. 1.4, which will be commented more in Chapter 7.
- **Other BSM particles:** Any long-lived particles beyond the SM spectrum, in addition to those discussed above, has a potential to become DM. Theoretically, some (almost-) exact discrete symmetries such as $\mathbf{Z}_2$ are employed for this purpose.
- **Particles with extra forces:** Except discrete symmetries, extra gauge interactions can also be considered belonging to the BSM. There have been many proposals for new gauge interactions, mainly working in the dark sector. The most well-known one is the dark force presented in [67]. Here, some stable elementary or composite particle can be a candidate for a DM particle.
- **ADM:** Conservation of asymmetric DM particles is similar to the conservation of baryon number B . So, one introduces a global symmetry $U(1)_{\text{ADM}}$ and follows the method of creating B in the standard Big Bang cosmology. It will be discussed in Chapter 8.
- **Wimpzilla:** In inflationary cosmology, reheating is the follow-up process. During the reheating process, some supermassive particles can be considered to be DM candidates which are called Wimpzillas [68].
- **Monopoles:** The following three items are discussed in Chapter 5, but for completeness, we also list them here. The monopole abundance is given by the Kibble mechanism, and the gauge symmetry breaking scale at a TeV scale can provide monopole DM.
- **Q balls:** Some Q balls, which are nontopological solitons, can be candidates of DM if they are stable. Global symmetries are the underlying symmetry because one needs large number of global charges in the Q ball scenario.
- **Primordial black holes:** This belongs to the next chapter, but for completeness, we show its summary here. Primordial black holes formed before nucleosynthesis and surviving now can work as DM portion in the cosmic energy pie. Based on the estimation on the density of these black holes, there is some constraint on this possibility.

Exercise

1. In Eq. (4.99), the left- and right-unitary matrices U^L and U^R are defined. For N families of quarks of the type (4.95), obtain the number of physical CP phases by considering the diagonalization of the u - and d -quark mass matrices without using U^R with non-diagonalized $M^{(d)}$.
2. Show that the integration of W with respect to the anticommuting variable $\int d^2\vartheta$ removes ϑ^0 and ϑ^1 terms and keeps only the coefficient of ϑ^2 term of W .

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Chapter 5

Extended Objects

Extended particles have a fixed size, while point-like particles are mathematical abstractions with zero size — Fermilab homepage

During the Universe evolution, scalar fields separated more than the horizon scale at that epoch are not correlated, and the random vacuum expectation values (VEVs) of scalar fields settle to some topological defects at a later epoch when the cosmic temperature is lowered. The temperature forming these defects defines the critical temperature of forming the defects. Zero-, one-, and two-dimensional defects are called monopoles, strings, and domain walls, respectively. Also, Q-balls have been considered. A monopole, having a finite size, may be considered to be a three-dimensional object, but we can consider it an approximate point particle. The scale of the approximate point particle is the inverse VEV. In this sense, we may distinguish an approximate point-like monopoles from Q-balls. Q-balls carrying multiple global charges can be considered large, and they may be regarded as three-dimensional objects. Also, black holes can be considered large three-dimensional objects.

Mathematically, they are classified by the homotopy group $\pi_n(M)$ where M is the coset space G/H for the symmetry breaking, $G \rightarrow H$, and n is the dimension of the mapped geometry [1],

$$\begin{aligned} \text{monopole } (d = 0): & \text{ nontrivial } \pi_2(M), \\ \text{string } (d = 1): & \text{ nontrivial } \pi_1(M), \\ \text{domain walls } (d = 2): & \text{ nontrivial } \pi_0(M). \end{aligned} \tag{5.1}$$

Spontaneous symmetry breaking discussed in Section 4.4 can realize the situations described in Eq. (5.1) [2]. In the standard model (SM) and grand unified theories (GUTs), spontaneous symmetry breaking is usually achieved by the

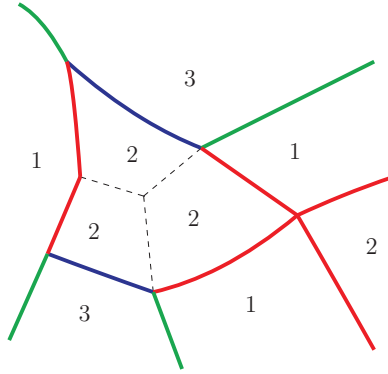


Fig. 5.1. Minima of Higgs VEVs in two dimensions.

VEVs of Higgs fields. In this case, topological defects presented in Eq. (5.1) depend on the number of components of the Higgs fields. In two-dimensional surface, we show VEVs of a real Higgs field ϕ in Fig. 5.1, where the potential has $\mathbf{Z}_3$ discrete symmetry. The potential with $\mathbf{Z}_3$ has three minima whose field values are marked as 1, 2, and 3, respectively. For field values of $0.5 < \phi < 1.5$, $1.5 < \phi < 2.5$ and $2.5 < \phi < 3.5$, minima can be considered to be 1, 2, and 3, respectively. Between two minima, there is a curve. In three dimensions, these boundary curves become domain walls [3].

5.1. Monopoles

Monopoles are classified as in Fig. 5.2. When we talk about monopoles here, it is considered to be zero-dimensional and the effective size of the probe is large, (probing length scale) $\gtrsim 1/(\text{VEV})$. The most familiar one is the topological defect formed when a simple or semi-simple gauge group without $U(1)$ is spontaneously broken to a subgroup with a $U(1)$ factor, which is the *'t Hooft–Polyakov monopole* [4]. The 't Hooft–Polyakov solution is a “magnetic monopole”. For that magnetic



Fig. 5.2. Types of monopoles. (a) Gauge theory monopole of 't Hooft and Polyakov, (b) global monopole, and (c) monopole attached to a flux of gauge field strength.

monopole with magnetic charge $g = \pm N/2e$ where N is an integer ($N = 1$ corresponds to the Dirac monopole with $|eg| = \frac{1}{2}$), the $\mathbf{B}$ flux lines go outward (inward) radially as shown in the left figure in Fig. 5.2. The mass of the 't Hooft–Polyakov monopole is

$$M_{\text{mono}} = \frac{\sqrt{4\pi}}{e} M_W C(\beta) = \frac{1}{\sqrt{\alpha_{\text{em}}}} M_W C(\beta), \quad (5.2)$$

where M_W is the charged gauge boson mass which is of order (gauge coupling) $\cdot$ (VEV), breaking simple or semi-simple group G at M_W down to $U(1) \times \dots$. In Eq. (5.2), $C(\beta)$ is of order 1 where $\beta = \lambda/e^2$ is the ratio of the quartic coupling and e^2 [4]. For a global monopole,¹ there is no flux lines as discussed in Section 4.5.

For the gauge monopole, one may consider further symmetry breaking, $U(1) \rightarrow \mathbf{Z}_N$ by a scalar field VEV $\langle \phi \rangle$ having the $U(1)$ quantum number N . Then, by gauge transformation one can push all $\mathbf{B}$ -field lines to the south pole, e.g., as shown in the right figure in Fig. 5.2. Because it arises from a gauge $U(1)$, the discrete monopole has the hair and the observer O of Fig. 4.4 judges that the discrete symmetry is not broken. On the other hand, if the discrete symmetry was obtained from a global $U(1)$, it was argued that there is no hair corresponding to some mother global symmetry. Nevertheless, recently it was shown that discrete hairs exist [5]. A global monopole is unstable because all global symmetries are approximate as discussed in Section 4.5 and it decays to lighter particles by interactions corresponding to the red of Fig. 4.5.

GUT monopoles have masses bigger than the GUT scale, presumably at the order 10^{16-17} GeV, which has led to the serious monopole problem [6]. This kind of GUT-scale monopoles was one of the reasons, proposing the inflationary cosmology [7]. For monopoles to behave like dark matter (DM), the estimate of their abundance is not by the decoupling temperature but by the Kibble mechanism. Thus, the gauge symmetry breaking scale must be of order TeV for it to look like DM.

5.2. Strings

One-dimensional defect is a *cosmic string* [1, 2]. It arises below the $U(1)$ symmetry breaking scale. If the mother simple or semi-simple group is a gauge (global) symmetry, the resulting string is called “*gauge (global) string*”. The tension of cosmic string or energy per length ($1/v$) is

$$\text{string tension} = O(v^2), \quad (5.3)$$

where v is the VEV, breaking the simple or semi-simple group.

Surrounding of a cosmic string is shown in Fig. 5.3: (a) for a gauge string and (b) for a global string. A gauge string does not have a wall attached to it. Therefore,

¹Here, “monopole” simply means zero-dimensional defect.

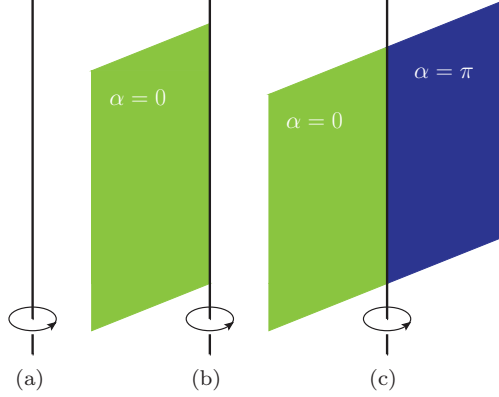


Fig. 5.3. The surrounding of a string: (a) a gauge string, (b) a global string with $N_{\text{DW}} = 1$, and (c) and a global string with $N_{\text{DW}} = 2$.

the energy of a string length L is only from the string core, i.e., the string tension times length, $O(v^2 L)$. A global string has walls attached to it and we must include the energy due to the attached walls to estimate the energy of a string length L , i.e., it is $E_{\text{core}} + E_{\text{wall}}$, where

$$E_{\text{core}} = O(v^2 L). \quad (5.4)$$

In reality, the logarithmic divergence is cut off because the horizon size is finite. At present, numerically E_{wall} exceeds E_{core} .

5.3. Domain walls

It is known that when a discrete symmetry is spontaneously broken then cosmic domain walls form [3]. The surface energy density of the global domain wall is

$$\text{surface energy density} = O\left(\frac{2\pi v^2}{r}\right), \quad (5.5)$$

where v is the VEV, breaking the mother global symmetry of the discrete group, and r is the distance from the core. If the mother continuous symmetry is gauged, the wall energy is zero because the kinetic energy density of scalar field far from the core is $|(i\vec{\nabla} - g\vec{A})\phi|^2$ with $\vec{A}$ chosen to make it vanish. For a global wall, we have instead

$$E_{\text{wall}} \approx L \int_{l_{\text{core}}}^{l_{\text{hor}}} \left| \frac{1}{r} \frac{d}{d\alpha} \phi \right|^2 2\pi r dr \simeq \pi L \frac{\mu^2}{\lambda} \ln \frac{l_{\text{hor}}}{l_{\text{core}}}, \quad (5.6)$$

where ϕ in Eq. (4.50) has been used. The surface energy density of a global wall has an effective thickness,

$$\lambda_{\text{thickness}} \approx \sqrt{\frac{\lambda}{2}} \frac{1}{\mu}, \quad (5.7)$$

where we used Eq. (4.50).

5.3.1. *Strings and domain walls*

Topological aspects of strings with domain walls are discussed above in Sections 5.2 and 5.3. When a compact (simple or semi-simple) group is broken spontaneously to a $U(1)$ symmetry, strings form. Furthermore, if the $U(1)$ is broken, domain walls form. As noted above, global domain walls carry wall energy. Strings with some domain walls are depicted in Fig. 5.3. A simple/semi-simple group breaking to $U(1)$ in three dimensions (3D) via VEVs of Higgs field is depicted in Fig. 5.3(a), $U(1)$ breaking to $\mathbf{Z}_1$ in Fig. 5.3(b), and $U(1)$ breaking to $\mathbf{Z}_2$ in Fig. 5.3(c). A gauge string with wall energy considered can be (a). Cases of the global strings with domain wall number $N_{\text{DW}} = 1$ and 2 can be considered as (b) and (c), respectively. Being continuous, the $U(1)$ group is used to get all information around a particle through the Gell-Mann–Levy equation (4.7) if the information at a nearby point is given, where one can distinguish the gauge and global strings by the existence of flux lines or not.

Continuous symmetry

For the monopole case, the flux lines of a gauge monopole are shown in Fig. 5.2(a). For the string case without a monopole attached to it, the flux lines of a gauge string can be consistent with the line symmetry of the type shown (in z -direction) in Fig. 5.3(a). There are two possible directions: one in the z -direction and the other in the radial directions from/to the line. Since the flux lines are continuous, we can consider flux lines around a gauge string coming from radial infinities to the string and goes out to $+\infty$ or $-\infty$ at the string, and vice versa. These possibilities are numerically achieved by the VEVs of the Higgs fields, a generalization of Fig. 5.1 in 3D, realizing the breaking a simple/semi-simple group to $SU(3) \times SU(2) \times U(1)$, where the monopole in the monopole solution is pushed to $+\infty$ or to $-\infty$. The Higgs field realizing this symmetry breaking respects the unbroken gauge group $U(1)$; thus we can introduce a phase to this Higgs field as discussed in Section 4.4. This phase is useful to discuss domain walls attached to a string.

Discrete symmetry

In a discrete symmetric theory with degenerate vacua, cosmological domain walls are created when the Universe cools down starting from a high temperature phase [3].

In field theory, it is usually modeled by the scalar field potential possessing a $U(1)$ symmetry. The $U(1)$ quantum number is normalized such that the smallest magnitude of nonvanishing quantum numbers is 1, i.e., that of ψ ,

$$\mathbf{Z}_N : \begin{cases} \psi \rightarrow e^{i\alpha} \psi, \\ \Phi \rightarrow e^{iN\alpha} \Phi. \end{cases} \quad (5.8)$$

Below the VEV of the scalar,² $\langle \Phi \rangle = f_a/\sqrt{2}$, the $U(1)$ symmetry is spontaneously broken down to $\mathbf{Z}_N$ by the following potential:

$$V \propto \lambda \left(\Phi^\dagger \Phi - \frac{f_a^2}{2} \right)^2. \quad (5.9)$$

Let us consider a heuristic case of $\mathbf{Z}_2$ for a global string. There are two possible vacua $|0\rangle$ and $|1\rangle$, corresponding to $q = 0, 1$ respectively, for the $\mathbf{Z}_2$ quantum number $e^{i\pi q}$. In Fig. 5.4, we present the case for $N_{\text{DW}} = 2$. In Fig. 5.4(a), we show that

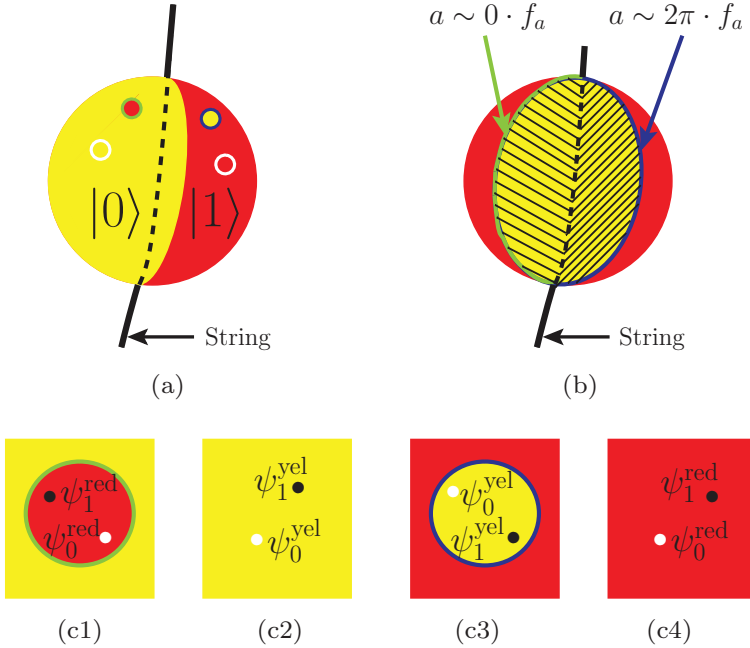


Fig. 5.4. The $\mathbf{Z}_2$ vacua. (a) There is a horizon-scale string. There are two distinct vacua, depicted as yellow and red. Particles in the $|\text{yel}\rangle \equiv |0\rangle$ and $|\text{red}\rangle \equiv |1\rangle$ vacua are also shown. (b) Domain walls are denoted as slashed. Walls will be colored limegreen and blue, depending on the viewing directions in the vacuum. These domain walls are attached to the horizon-scale string. (c) Figures (c1) and (c3) depict *DW*-balls, colored limegreen and blue, and (c2) and (c4) show the particles in the vacua. Particles ψ_i^A ($i = 0, 1$; $A = \text{yel}, \text{red}$) are in the Higgs vacuum $|A\rangle$.

²Fermion fields are assumed not developing VEVs to preserve the Lorentz symmetry.

there are two vacua colored yellow ($\equiv |0\rangle$) and red ($\equiv |1\rangle$). If they arise from high temperature in an ultraviolet completed theory, a string is present. Around the string two kinds of domain walls are attached, which we distinguish by the colors: limegreen (between red and yellow) and blue (between yellow and red). These two colors can be considered two colors of the opposite surfaces of the domain wall.³ Angles for these two walls are connected to 0 and π , respectively, as shown in Fig. 5.3(c). For the phase $N\alpha$ of Φ in (5.8), we can represent it as a/f_a , i.e., the range of a is

$$0 \leq a < 2\pi N f_a. \quad (5.10)$$

In Fig. 5.4(b), they are shown with slashed lines viewed from the wedged yellow vacuum. Since topology is the only important aspect, the wedged $|0\rangle$ vacuum of Fig. 5.4(b) instead of the half sphere walls does not lose the generic feature of the string-wall system.

The quantum field Ψ_q has a $\mathbf{Z}_2$ quantum number $q = 0, +1$ modulo 2: $P\Psi_q P^{-1} = e^{i\pi q} \Psi_q$ whose wave functions in the $|\text{yel}\rangle$ and $|\text{red}\rangle$ vacua are given by

$$\psi_0^{\text{yel}}(x) = \langle \psi_0; \text{yel} | \Psi_0(x) | \text{yel} \rangle, \quad (5.11)$$

$$\psi_1^{\text{yel}}(x) = \langle \psi_1; \text{yel} | \Psi_1(x) | \text{yel} \rangle, \quad (5.12)$$

$$\psi_0^{\text{red}}(x) = \langle \psi_0; \text{red} | \Psi_0(x) | \text{red} \rangle, \quad (5.13)$$

$$\psi_1^{\text{red}}(x) = \langle \psi_1; \text{red} | \Psi_1(x) | \text{red} \rangle, \quad (5.14)$$

where $|\text{yel}\rangle \equiv |0\rangle$ and $|\text{red}\rangle \equiv |1\rangle$. For example, $\psi_1^{\text{red}}(x)$ is the wave function of a $\mathbf{Z}_2$ odd particle in the $|\text{red}\rangle$ vacuum. Also, ψ_1 can be localized in the wall, which however is not considered here.

The string-wall system also allows the isolated balls shown in Fig. 5.4(c1) and 5.4(c3). The particles with $\mathbf{Z}_2$ quantum numbers 0 and 1 can be present, which are shown in Figs. 5.4(c1)–(c4). The *DW-hole*, the opposite vacuum (e.g. $|\text{red}\rangle$) inside a vacuum (e.g. inside $|0\rangle \equiv |\text{yel}\rangle$ vacuum) as shown in Fig. 5.5, can be present even though its formation in a late phase of the Universe evolution is energetically unflavored, with a string loop or without the loop.

The potential of the phase field a of Φ in (5.8) and (5.10) is flat with the exact $U(1)$ invariance of Eq. (5.8). In an ultraviolet completed theory, the global $U(1)$ invariance is an accidental symmetry and broken by higher order terms [8, 9], as shown in Figs. 4.4 and 4.5. Let us parameterize the potential $V[\alpha]$ for the global

³For the $N_{\text{DW}} = 1$ case, the opposite surfaces of the domain wall has the same color.

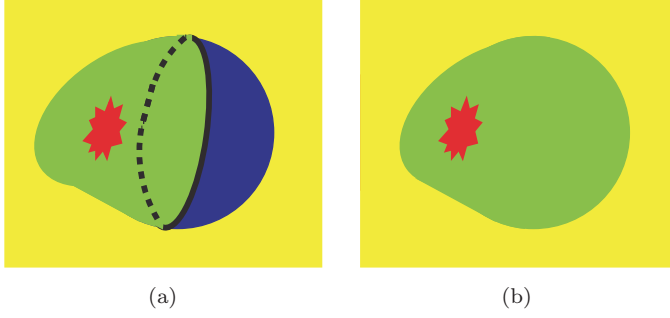


Fig. 5.5. Details of Fig. 5.4(c1): (a) with a closed string and (b) without a closed string.

$U(1)$ in terms of the phase field $a \equiv N_{\text{DW}} f_a \alpha$ as⁴

$$\frac{\delta m^2}{M^2} f_a^4 \left(\frac{1 - e^{i\alpha}}{2} + \text{h.c.} \right) = \frac{\delta m^2}{M^2} f_a^4 \left(1 - \cos \frac{a}{f_a} \right). \quad (5.15)$$

For $N_{\text{DW}} = 2$ the range of a is defined as $a = [-2\pi f_a, +2\pi f_a]$ for $\alpha = [-2\pi, +2\pi]$. The height of the potential of a is typically given by a leading $U(1)$ breaking term.⁵

For two $\mathbf{Z}_2$ odd particles, we consider that sum of these two does not carry any $\mathbf{Z}_2$ charge,

$$\mathbf{Z}_2 : \psi_1 \psi'_1 \rightarrow (-)(-)\psi_1 \psi'_1 = \psi_1 \psi'_1. \quad (5.16)$$

The DW-balls are shown in more detail in Figs. 5.4(c1) and 5.4(c3), where several particles are present inside the DW-balls. Figures 5.4(c2) and 5.4(c4) show particles in the $|\text{yel}\rangle$ and $|\text{red}\rangle$ vacua. ψ_0 does not carry the discrete quantum number. Therefore, to check the violation of discrete symmetry, we consider only the disappearance of $\mathbf{Z}_2$ odd-type particles, i.e., ψ_1 . Due to Eq. (5.16), for the odd number of ψ_1 particles inside the DW-hole, it is sufficient to consider disappearance of one ψ_1 .

Collision of DW-ball with a large wall

It has been known that domain walls arising from the Peccei–Quinn symmetry with $N_{\text{DW}} \geq 2$ carry too much energy at present in the standard Big Bang cosmology [11]. For the Peccei–Quinn symmetry with $N_{\text{DW}} = 1$, domain walls attached to a horizon-scale string looks like Fig. 5.6. In (a), a large wall attached to a horizon-scale string is shown. There are also a scale invariant spectrum of wall disks surrounded by strings. In (b), a disk is shown to punch the large wall, creating a vacant hole which

⁴For the quantum chromodynamics (QCD) axion [10], $\delta m^2 f_a^4 / M^2 = f_\pi^2 m_\pi^2 \sqrt{Z} / (1 + Z)^2 \approx \Lambda_{\text{QCD}}^4$ where $Z = m_u / m_d$.

⁵The anomaly term can be a leading term in some cases, as in the QCD axion case.

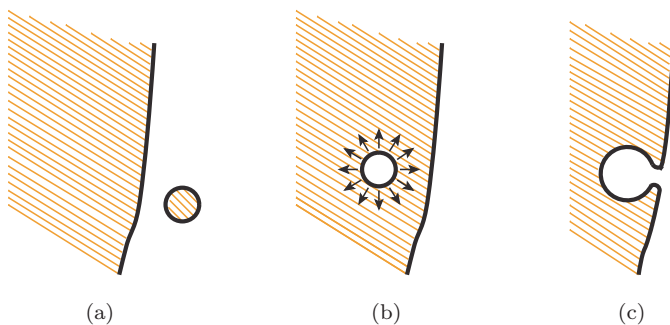


Fig. 5.6. The horizon-scale string-wall system with $N_{\text{DW}} = 1$ with spontaneously broken $\mathbf{Z}_1$: (a) a large wall attached to the string and a disk of wall, (b) the disk punching the large wall, and (c) the hole (a kind of DW-ball) in the large wall expands with velocity $\approx c$ [12, 13].

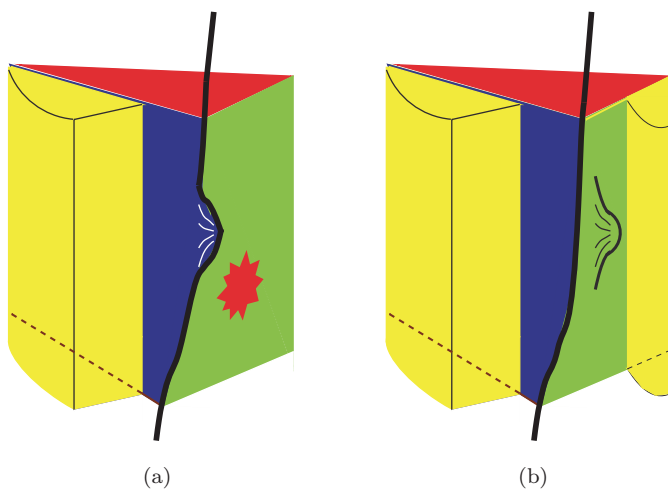


Fig. 5.7. The small DW-balls of Fig. 5.5 colliding with a large wall. Collisions of (a) and (b) of Fig. 5.5 are depicted.

expands with the light velocity, and erases the horizon-scale string-wall system as shown in (c). So, it is argued that $N_{\text{DW}} = 1$ does not have a serious cosmological problem [12, 13].

However, cases with $N_{\text{DW}} \geq 2$ have cosmological problems [11]. For the case of $N_{\text{DW}} = 2$, similarly to a small ball of Fig. 5.6, small balls bounded by a string-wall and just a wall are shown in Figs. 5.5(a) and 5.5(b), respectively. After the collisions of these small DW-balls of $\mathbf{Z}_2$ with a large wall, the large wall is not erased as shown in Figs. 5.7(a) and 5.7(b).

Theoretical models for the domain wall solution

There are theoretical solutions of the above cosmic domain wall problem. Mainly, the problem has been discussed in the QCD axion solutions, which can be applied to other domain wall models.

An axion solution may arise from a GUT theory. As an example, let us consider an $SU(N)$ GUT. Then suppose that a naive calculation of the domain wall number gives n . But, the center of $SU(N)$, i.e., N , is unbroken even if $SU(N)$ is broken. So, N vacua among n vacua can be identified by this unbroken discrete group. Therefore, the number of physically distinguishable vacua is n/N which is called the Lazarides–Shafi mechanism [14]. Here, a part of the gauge symmetry is used, and hence there is no wall energy between the identified vacua.

There is another method to identify some vacua by unbroken discrete groups. The most useful one is an unbroken discrete group of a global $U(1)$, which can be called the Choi–Kim mechanism [15]. Consider the case that the final global $U(1)$ is $U(1)_{PQ}$. In Fig. 5.8, we consider two directions of $U(1)$ ’s, but one direction represented as solid arrows is broken. Namely, we consider two $U(1)$ ’s among which one combination is $U(1)_{PQ}$. The $U(1)_{PQ}$ carries all the QCD anomaly, and the other $U(1)$ we consider is denoted as $U(1)_{Gold}$. The $U(1)_{Gold}$ does not carry any gauge anomaly. If out of two $U(1)$ ’s one is global and the other is gauged, then $U(1)_{Gold}$ is the longitudinal direction of some gauge boson. In this case, if it is spontaneously broken, there is no Goldstone boson but the discrete subgroup of $U(1)_{Gold}$ can be used to identify the axion vacua. This is shown in Fig. 5.8 where we introduced two $U(1)$ ’s with two $U(1)$ domain wall numbers, $N_1 = 3$ and $N_2 = 2$, where there are six vacua (red bullets). Six vacua are connected by the Goldstone boson direction (limegreen line); in fact by the discrete subgroup of $U(1)_{Gold}$. In this case, the physically distinguishable vacua is the largest common divisor of N_1 and N_2 , and Fig. 5.8 gives $N_{DW} = 1$ by the Choi–Kim mechanism. The choice of arrows in Fig. 5.8 is dictated by a ratio of VEVs of Higgs field [32].

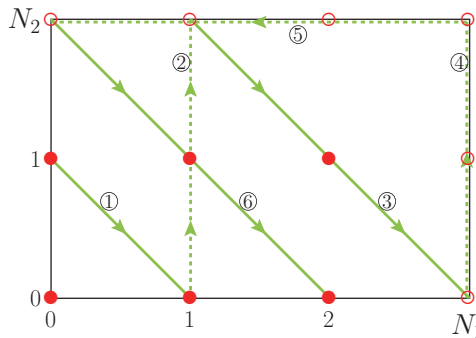


Fig. 5.8. The Choi–Kim mechanism. The Goldstone boson direction is arrowed lines and the torus identification is dashed arrowed lines. The arrows along the circled numbers identify all six bulleted vacua.

There is another method to alleviate the domain wall problem by positing the existence of a new confining force [16]. The instantons of this force can generate an axion potential that erases the horizon-scale axion strings, as we discussed in Fig. 5.6 by replacing the QCD wall by the wall due to the new confining force, long before QCD effects become important. The walls generated by the new confining force would decay as discussed in Fig. 5.6. When the QCD phase transition occurs at temperature around GeV, there is no horizon-scale strings for the QCD walls to be attached [16].

$U(1)_{\text{anom}}$ global symmetry

Related to the N_{DW} , there is an interesting compactification in string theory. Note that there are some compactifications of the heterotic string where $U(1)_{\text{anom}}$ appears. It means that a $U(1)$ subgroup of $E_8 \times E_8'$ survives in the compactification process. Note also that there always exists the model-independent (MI) axion in the compactification of ten dimensions (10D) to four dimensions (4D). The MI axion is the direction from a global symmetry in 4D. $U(1)_{\text{anom}}$ is a gauge direction in 4D. So, it is exactly the Choi–Kim mechanism discussed above and realized in string compactification [17, 18]. It is based on the 't Hooft mechanism discussed in Section 4.4.4. Because $N_1 = 1$ [18, 19] and usually $N_2 = \text{huge integer}$, we obtain $N_{\text{DW}} = 1$. This conclusion for $N_{\text{DW}} = 1$ is not automatic but depends on the ratios of VEVs such that all vacua are identified [32].

If there is no $U(1)_{\text{anom}}$ present in the string compactification, the MI axion is the physical degree whose decay constant is of order the GUT scale. Its point is shown as the white square in the upper-left corner of Fig. 9.11.

5.4. Q-balls

In the previous subsections, we considered topological defects, played by the VEVs of Higgs fields. There also exist nontopological defects called *Q-balls* in scalar field theories possessing a global $U(1)$ symmetry [21–23], arising in the process of spontaneous symmetry breaking of the global symmetry. These objects can be viewed as coherent states of the scalar field with a large number of $U(1)$ charges. Since a large number of charges are relevant in cosmological applications, the size of a Q-ball can be considered to be large, i.e., as a three-dimensional defect. The reason for such $U(1)$ symmetries in the SM can be baryonic or leptonic charge. In supersymmetric extensions of the SM, the scalar superpartners of baryons or leptons can form coherent states with a fixed baryon or lepton number, making the existence of Q-balls possible. These can be stable because of the energy consideration for a fixed number of conserved charges, forbidding their decaying to free particles. They are not included in Eq. (5.1) because of their nontopological nature.

Scalar fields with B and L global quantum numbers are numerous in supersymmetric extension of the SM. Therefore, many studies on Q-balls are modeled in supersymmetry [25].

From Eqs. (4.31) and (4.32), the conserved charge of ϕ for the continuous parameter $\alpha/2$ is

$$Q = \frac{1}{2i} \int d^3x (\phi^* \partial_t \phi - \phi \partial_t \phi^*). \quad (5.17)$$

With this definition, Q is an even integer. A Lagrange multiplier ω is used in the functional of energy to guarantee the charge

$$E_\omega = E + \omega \left[Q - \frac{1}{2i} \int d^3x (\phi^* \partial_t \phi - \phi \partial_t \phi^*) \right], \quad (5.18)$$

which can be rewritten as

$$E_\omega = \int d^3x \left[\frac{1}{2} |\dot{\phi} - i\omega\phi|^2 + \frac{1}{2} |\vec{\nabla}\phi|^2 + \hat{U}_\omega(\phi, \phi^*) \right], \quad (5.19)$$

where

$$\hat{U}_\omega = U - \frac{1}{2} \omega^2 \phi^2. \quad (5.20)$$

The first term of (5.19) is minimized for

$$\phi = \phi_0(\mathbf{x}) e^{i\omega t}, \quad (5.21)$$

where $\omega = 0$ gives E and potential energy $U(\phi, \phi^*)$ of Eqs. (5.18) and (5.20).

The interesting region of ω is [22],

$$\omega_- \leq |\omega| \leq \omega_+, \quad (5.22)$$

where $\omega_-^2 = \min|2U/\phi^2|_{\phi_+(\omega_-)} \geq 0$ where $\phi_+(\omega_-)$ is the nonzero value of ϕ where $U_\omega(\phi_+(\omega))$ is minimized, and $\omega_+^2 = \partial^2 U / \partial \phi^2|_{\phi=0}$. We also define a ϕ outside of (5.22),

$$\phi_0(\omega) = \phi(0). \quad (5.23)$$

A Q-ball solution is stable at any values of $\phi^* \phi$ at which $U(\phi, \phi^*)$ is less than $m^2 \phi^* \phi$, viz. the number operator of ϕ quanta is $a^\dagger a$. It means that the static energy of Q-ball solution per unit charge is less than m , implying that the Q-ball cannot decay to a gas of free particles.

5.4.1. Thin wall Q-ball

The energy profile of Q-ball is concentrated in the surface if $\phi_0(\mathbf{x})$ of (5.21) takes the following form [21]:

$$\phi_0(\mathbf{x}) = \theta(R - r) \phi_0. \quad (5.24)$$

Then, from Eq. (5.17) we obtain the charge Q inside the thin Q-ball volume V as $Q = \omega \phi_0^2 V$. Then, Eq. (5.18) gives

$$E_V = \frac{Q^2}{2\phi_0^2 V} + U(\phi_0)V, \quad (5.25)$$

which is minimized for $V = \sqrt{Q^2/2U(\phi_0)\phi_0^2}$, leading to

$$E = \sqrt{\frac{2U(\phi_0)}{\phi_0^2}} Q. \quad (5.26)$$

In terms of parameters of (5.22) and (5.23), the region is

$$\omega \simeq \omega_- \quad \text{or} \quad \phi_0(\omega) \sim \phi_+(\omega). \quad (5.27)$$

5.4.2. Thick wall Q-ball

In terms of parameters of (5.22) and (5.23), the thick wall Q-ball is for

$$\omega \simeq \omega_+ \quad \text{or} \quad \phi_0(\omega) \sim \phi_-(\omega), \quad (5.28)$$

whose effects were presented in Refs. [22, 24].

5.4.3. Gauged Q-ball

So far the U(1) symmetries related to the Q-balls were global symmetries. Local U(1) symmetries can lead to Q-balls also, which are called gauged Q-balls. Such Q-balls become unstable for large values of their charge because of the repulsion mediated by the gauge force. However, small Q-balls can still exist.

But, the repulsion can be made weak through the presence of fermions with charge opposite to that of the scalar condensate in the interior of the Q-ball. For this to work, the fermions must carry an additional conserved quantum number such that their annihilation is prevented. This scenario can lead to the existence of large Q-balls. Such a scenario for a large gauged Q-ball is discussed in [26].

5.5. Primordial black holes

A recent estimate of the primordial black holes (PBHs) has been given in [27], which attracted a great deal of attention after the LIGO discovery of GW150914 [28]. When there was a great compression of energy in the early Universe, the mass of a PBH is estimated as

$$M_{\text{PBH}} \sim \frac{c^3 t}{G_N} \sim 10^{15} \left(\frac{t}{10^{-23} \text{ s}} \right) \text{ g}, \quad (5.29)$$

where t corresponds to the reheating epoch or the time at which the characteristic PBH scale reenters the horizon in the inflationary context or to the time of the

relevant cosmological phase transition, depending on the PBH formation scenarios [29]. Some interesting masses guessed from (5.29) are for those formed at 1 s which would be as large as $10^5 M_\odot$, and for those formed at the present epoch which would give $\gtrsim M_\odot$.

5.6. Axion mini-clusters

Mini-clusters formed with axions below the Universe temperature 1 GeV were considered in [30]. The original mass estimate of the miniclusters was about $10^{-9} M_\odot$, which can be taken as an order of magnitude estimate. A recent study on microlensing pinpoints to the mini-cluster mass around $10^{-10} M_\odot$ [31]. If axion mini-clusters carry most of axion energy density of the Universe now, then it is more difficult to detect cosmic axions unless Earth passes through the axion mini-clusters. It is not a kind of soliton because its energy derives from the oscillating classical field. So, we do not include it here but consider it a part of the axion energy density.

5.7. Extended objects as DM

Among the extended objects, strings and domain walls cannot act like DM. But, monopoles, PBHs, and Q-balls can behave like DM.

- **Monopoles:** The estimate of monopole abundance is not by the decoupling temperature but by the Kibble mechanism [2]. Thus, the gauge symmetry breaking scale must be of order TeV for it to behave like DM.
- **Q-balls:** Some Q-balls, which are nontopological solitons, can be candidates of DM if they are stable. Global symmetries are the underlying symmetry because one needs large number of charges in the Q-balls.
- **PBHs:** PBHs formed before nucleosynthesis and surviving now can work as DM portion in the cosmic energy pie. At present, PBHs are not ruled out completely, but there is a tension for PBHs to work as meaningful cold DM because of the successful nucleosynthesis data.

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Chapter 6

Bosonic Collective Motion

*All logical arguments can be defeated by the simple refusal
to reason logically — Steven Weinberg*

In this chapter, we discuss the bosonic collective motion (BCM). The BCM is a quite general concept. Since axion is the prototype model for the BCM, symmetry principles are the key to (almost) stable dark matter (DM) candidates. In this chapter, we discuss BCM arising from the approximate global symmetries, and in Chapter 7, we will discuss cold dark matter (CDM) from discrete symmetries. These symmetries are affected by gravity, which we call “gravity spoil” of symmetries. Gravity spoil of global symmetries has already been mentioned in the preceding chapter, and we will summarize it in Section 6.6 before using the discrete symmetries in Chapter 7.

6.1. BCM

Bosonic collective or coherent motion can be CDM, depending on its mass and couplings. It was first pointed out in [1] in connection with the “invisible” axion couplings [2–5]. The zeroth requirement is that it has lived until now with lifetime greater than the age of the Universe t_U . For the quantum chromodynamics (QCD) axion, it translates to mass being smaller than ~ 20 eV. We will use the letter C in BCM for both “collective” and “coherent” in the sense that the classical motion of the scalar is that the individual particles move with the same magnitude of velocity (collective) and also in some cases in the same quantum state (coherent). A real pseudoscalar or scalar field ϕ has an effective potential of the form

$$V = \frac{m_0^2}{2}\phi^2 + \frac{\lambda}{4}\phi^4 + (\cdots). \quad (6.1)$$

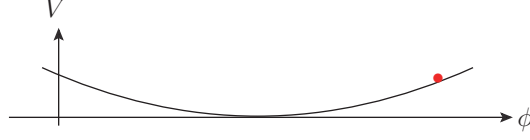


Fig. 6.1. A potential shape of ϕ . The red bullet corresponding to t_{BCM} is at the time of $m = 3H$.

In some region of ϕ value, where $\lambda\phi^2 \ll m_0^2$, we can consider only the mass term.

At some time in the late Universe, $m_0 \simeq H$ will be satisfied, which is the beginning of ϕ field oscillation. Let the beginning time of the oscillation be t_{BCM} . Figure 6.1 shows a bullet representing the same value $\langle\phi\rangle$ in the region inside the horizon scale. After inflation, the regions within scale of quantum fluctuation are correlated. But before t_{BCM} , the classical field $\langle\phi\rangle$ stays at the bullet.¹ For $t > t_{\text{BCM}}$, $\langle\phi\rangle$ rolls down and oscillates around the minimum with frequency m . Then, the energy density (kinetic energy plus potential energy) due to this bullet oscillation averaged over one cycle is

$$\langle\rho\rangle = \frac{1}{2}\langle\dot{\phi}\rangle^2 + \frac{m_0^2}{2}\langle\phi\rangle^2,$$

which is like harmonic oscillator motion in quantum mechanics. If oscillation rate is smaller than the Hubble expansion rate $m \lesssim H$, there is only the potential energy V . On the other hand, if the oscillation rate is greater than the Hubble expansion rate, $m \gtrsim H$, the bullet oscillation shown in Fig. 6.1 contains both potential and kinetic energies. This was introduced in Section 2.6.4.

Example 6.1 (Massless scalar). If m were vanishing, a massless scalar with $(\lambda/4)\phi^4$ coupling satisfies $\ddot{\phi} = -3H\dot{\phi} - \lambda\phi^3$. The energy density is

$$\begin{aligned}\rho &= \frac{1}{2}\dot{\phi}^2 + \frac{\lambda}{4}\phi^4, \\ \dot{\rho} &= \dot{\phi}(-3H\dot{\phi} - \lambda\phi^3) + \lambda\phi^3\dot{\phi} = -3H\dot{\phi}^2,\end{aligned}$$

which gives

$$\dot{\rho} + 3H\dot{\phi}^2 = \dot{\rho} + 6H\rho + H\left(-\frac{3\lambda}{2}\phi^4\right) = 0,$$

or

$$\begin{aligned}\frac{1}{R^3}\frac{d}{dt}(\rho R^3) &= \dot{\rho} + 3H\rho = H\frac{3\lambda}{2}\phi^4 - 3H\rho \\ &= 3H\rho - 3H\dot{\phi}^2 = 3H\left(\frac{\lambda}{4}\phi^4 - \frac{1}{2}\dot{\phi}^2\right),\end{aligned}$$

where R is the scale factor.²

¹We will distinguish the classical field and the BCM quantum by $\langle\phi\rangle$ and a_{quantum} , respectively.

²In this chapter on axions, we use R for the scale factor to distinguish it from the axion field a .

An exactly massless boson is presumably arising from a spontaneously broken global symmetry. But, as discussed in Chapter 4, global symmetries are only approximate. So, for all bosons, we must consider the mass terms. So, let us discuss the evolution of a pseudo-Goldstone boson which is created below the scale f by breaking the global symmetry spontaneously. The dominant explicit breaking strength is parameterized by Λ^4 which is in the red part of Fig. 4.5. So, let us consider the action

$$\int \sqrt{-g} \left(-\frac{1}{2} \partial_\mu \phi \partial^\mu \phi + \frac{\Lambda^4}{2} \left[\cos \frac{\phi}{f} - 1 \right] \right).$$

The field ϕ satisfies the following equation in the evolving homogeneous and isotropic Universe, i.e., with the FLRW metric:

$$\ddot{\phi} + 3H \dot{\phi} + \frac{f}{2} m_0^2 \sin \frac{\phi}{f} = 0, \quad \text{Periodicity: } \phi \rightarrow \phi + 2\pi f, \quad (6.2)$$

where $m_0^2 = \frac{\Lambda^4}{2f^2}$. Now, we have

$$\rho = \frac{1}{2} \dot{\phi}^2 + \frac{\Lambda^4}{2} \left[1 - \cos \frac{\phi}{f} \right]. \quad (6.3)$$

With $H = 0$, there results the sine-Gordon equation,

$$\frac{d^2}{dt^2} \frac{\phi}{f} + \frac{m_0^2}{2} \sin \frac{\phi}{f} = 0, \quad \text{with } m_0 = \frac{\Lambda^2}{\sqrt{2}f}. \quad (6.4)$$

To start at $\phi/f < \pi$, we consider

$$\frac{\phi}{f} = 2 \tan^{-1} e^{-m_0(t+c)}, \quad c < 0 \text{ for anharmonic region at } t = 0. \quad (6.5)$$

For $c = 0$, this solution connects $\phi = \pi f$ at $t = 0$ to $\phi = 0$ at $t = \infty$. So, this form cannot be used as an oscillatory solution in the evolving Universe. Thus, we need a scheme to go into the linearization of the differential equation (6.2).

6.1.1. Linearization: The bottleneck period

The linearization occurs when the Hubble friction term is more important than the mass term. As the Universe cools down, the Hubble parameter H approaches m_0 from above. At some point, therefore, we must include the dissipation term. Note that the second derivative in Eq. (6.4) brings down $-m_0^2$ in front of $\sin(\phi/f)$ to satisfy the equation.

To see the bottleneck period from Eq. (6.2), consider

$$\ddot{\theta} + 3H\dot{\theta} + \frac{m_0^2}{2} \sin \theta = 0, \quad (6.6)$$

where $\phi = f_a \theta$. Let us introduce a conformal time $\tau(t)$ as a function of t such that the first derivative term of θ with respect to τ in the differential equation (6.6) is

absent. Then, we obtain

$$\theta'' + \frac{m^2}{\dot{\tau}^2} \sin \theta = 0, \quad (6.7)$$

where prime denotes the derivative with respect to τ and $\ddot{\tau}/\dot{\tau} = -3H$, and³

$$m^2 = \frac{m_0^2}{2}. \quad (6.8)$$

Since R has a power law with respect to t in the radiation-dominated (RD) and matter-dominated (MD) Universes, let us parameterize it as $H = n/t$. Then,

$$\begin{aligned} \dot{\tau} &= \exp \left[-3 \int^t H(t') dt' \right] \\ &= \begin{cases} e^{-3Ht} & \text{for constant } H, \\ (t/t_0)^{-3n} & \text{with } n = \frac{1}{2} \text{ in RD and } n = \frac{2}{3} \text{ in MD.} \end{cases} \end{aligned} \quad (6.9)$$

Thus,

$$\tau = \begin{cases} -\frac{1}{3H} e^{-3Ht} & \text{for constant } H, \\ \frac{t_0}{1-3n} (t/t_0)^{-3n+1} & \text{with } n = \frac{1}{2}, \frac{2}{3} \text{ respectively in RD and MD,} \end{cases} \quad (6.10)$$

which gives

$$-2t_0 \left(\frac{t}{t_0} \right)^{-1/2} \quad \text{and} \quad -t_0 \left(\frac{t}{t_0} \right)^{-1}$$

in the RD and MD Universes, respectively. In terms of τ , Eq. (6.7) is parameterized in terms of n as, in the RD and MD Universes,

$$\theta'' + \frac{m^2}{\left[(3n-1)^2 \left(\frac{\tau}{t_0} \right)^2 \right]^{\frac{3n}{3n-1}}} \sin \theta = 0. \quad (6.11)$$

Note that, for the parameterization $H = n/t$, the t range $(0, +\infty)$ is mapped into $(-\infty, 0)$.

³The linearization occurs at the cosmic temperature somewhat below 1 GeV and we will treat m_0 constant just to show the bottleneck problem analytically.

Approximate solution in the linearization regime

When θ falls down to a sufficiently small value, we can approximate $\sin \theta \simeq \theta$, and Eq. (6.11) is simplified to

$$\theta'' + \bar{m}^2 \theta = 0, \quad (6.12)$$

where

$$\bar{m}^2(\tau) = \frac{m^2}{\left[(3n-1)^2 \left(\frac{\tau}{t_0} \right)^2 \right]^{\frac{3n}{3n-1}}}. \quad (6.13)$$

In the limit $\tau \rightarrow -\infty$, θ approaches a constant θ_0 . The linearization solution is to disregard this constant and we expand the linearization solution as descending functions of θ_k

$$\theta(\tau) = \sum_{k=0}^{\infty} \theta_k(\tau). \quad (6.14)$$

Assuming $\bar{m}(\tau)$ is sufficiently small compared to τ^{-1} , we obtain recursion relations,

$$\begin{aligned} \theta_1'' &= -\bar{m}^2(\tau) \theta_0 \\ \theta_2'' &= -\bar{m}^2(\tau) \theta_1(\tau) \\ &\vdots \\ \theta_{k+1}'' &= -\bar{m}^2(\tau) \theta_k(\tau), \end{aligned}$$

and the Neumann series solution is

$$\theta_{k+1}(\tau) = - \int_{-\infty}^{\tau} d\tau' \int_{-\infty}^{\tau'} d\tau'' \bar{m}^2(\tau'') \theta_k(\tau''). \quad (6.15)$$

Since θ_0 is taken as a constant, $\theta_k(\tau)$ can be expressed as a multiple integral,

$$\begin{aligned} \theta_k(\tau) &= \theta_0 \int_{-\infty}^{\tau} d\tau_{2k} \int_{-\infty}^{\tau_{2k}} d\tau_{2k-1} [-\bar{m}^2(\tau_{2k-1})] \\ &\quad \times \int_{-\infty}^{\tau_{2k-1}} d\tau_{2k-2} \int_{-\infty}^{\tau_{2k-2}} d\tau_{2k-3} [-\bar{m}^2(\tau_{2k-3})] \\ &\quad \times \cdots \times \int_{-\infty}^{\tau_3} d\tau_2 \int_{-\infty}^{\tau_2} d\tau_1 [-\bar{m}^2(\tau_1)] \\ &= (-1)^k \theta_0 \left\{ \prod_{j=1}^k \int_{-\infty}^{\tau_{2j+1}} d\tau_{2j} \int_{-\infty}^{\tau_{2j}} d\tau_{2j-1} [\bar{m}^2(\tau_{2j-1})] \right\}_{\tau_{2k+1}=\tau}. \end{aligned} \quad (6.16)$$

For $n > \frac{1}{3}$, with $\alpha = 1/(3n - 1)$, θ_k is given by

$$\theta_k(\tau) = \theta_0 \frac{\Gamma(\frac{1}{2\alpha} + 1)}{\Gamma(k+1)\Gamma(\frac{1}{2\alpha} + k+1)} \left[-\frac{1}{4} m^2 t_0^2 \left(\frac{|\tau|}{\alpha t_0} \right)^{-2\alpha} \right]^k, \quad (6.17)$$

$$\theta_k(t) = \theta_0 \frac{\Gamma(\frac{1}{2\alpha} + 1)}{\Gamma(k+1)\Gamma(\frac{1}{2\alpha} + k+1)} \left[-\frac{1}{4} m^2 t^2 \right]^k. \quad (6.18)$$

By Mathematica, one can sum the series to find a hypergeometric function,

$$\theta(t) = {}_0F_1 \left(\frac{1}{2\alpha} + 1, -\frac{1}{4} m^2 t^2 \right) \theta_0. \quad (6.19)$$

Approximate solution in the (anharmonic) nonlinear regime

With the trick shown above, let us now study the region with a large value of θ_0 , i.e., in a deep anharmonic regime,

$$\theta_0 \gg \sum_{k=1}^{\infty} \theta_k(\tau). \quad (6.20)$$

Then, $\sin(\theta_0 + \sum_{k=1} \theta_k(\tau)) \simeq \sin \theta_0 + \cos \theta_0 \sum_k \theta_k$. Thus, the recursion relations are

$$\begin{aligned} \theta_1'' &= -\bar{m}^2(\tau) \sin \theta_0 \\ \theta_2'' &= -\bar{m}^2(\tau) \cos \theta_0 \theta_1(\tau) \\ &\vdots \\ \theta_{k+1}'' &= -\bar{m}^2(\tau) \cos \theta_0 \theta_k(\tau), \end{aligned}$$

$$\begin{aligned} \theta_k(\tau) &= (-1)^k \theta_0 \cos^{k-1} \theta_0 \sin \theta_0 \\ &\times \left\{ \prod_{j=1}^k \int_{-\infty}^{\tau_{2j+1}} d\tau_{2j} \int_{-\infty}^{\tau_{2j}} d\tau_{2j-1} [\bar{m}^2(\tau_{2j-1})] \right\}_{\tau_{2k+1}=\tau}. \end{aligned} \quad (6.21)$$

An asymptotic solution is expressible in terms of a hypergeometric function,

$$\theta(t)_{\text{asymptotic}} = \theta_0 - \tan \theta_0 \left[-1 + {}_0F_2 \left(\frac{1}{2\alpha} + 1, -\frac{1}{4} m^2 t^2 \cos \theta_0 \right) \right]. \quad (6.22)$$

Two solutions given in Eqs. (6.19) and (6.22) are shown in Fig. 6.2, in blue and red colors, together with the numerical solution of [7]. We can express the solution in the entire region by two hypergeometric functions by joining two at a reasonable θ_2 where the analytic solutions almost match the numerical solution.

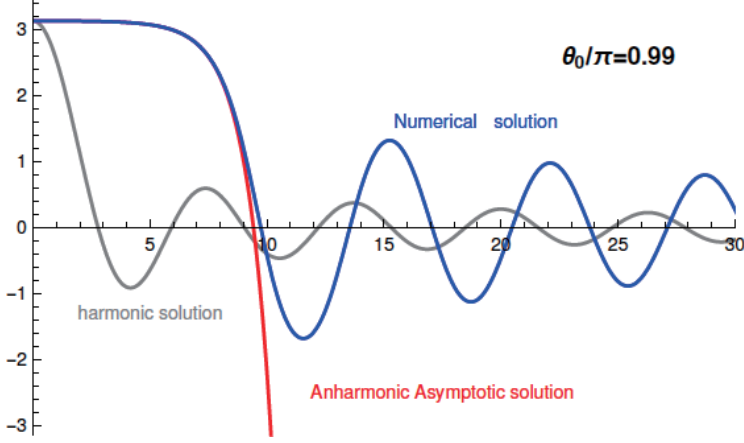


Fig. 6.2. The numerical solution (blue) in the anharmonic regime $\theta_0 = 0.99\pi$ [6].

As an illustration, let us consider that $\Phi = \frac{\pi}{8}$ is sufficiently small to consider for $\sin \Phi \rightarrow \Phi$, this happens for

$$t_2 + c \simeq \frac{-\ln(\pi/32)}{m - H} \approx \frac{2.3}{m} \quad \text{for } H \ll m. \quad (6.23)$$

The t_2 -form, Eq. (6.23), is taken as the commencement time of BCM oscillation $t_2 \simeq 3m^{-1}$, with a sufficiently small Φ : $\Phi(t_2) \ll 1$, e.g., less than $\pi/8$. From this time on, a linear approximation of (6.7) is valid:

$$\ddot{\Phi} + m^2\Phi \simeq 0. \quad (6.24)$$

Then, the oscillation of $f\Phi$ is CDM. Now, we can take $t_2 \simeq 3m^{-1}$, which is at a later time than the customary commencement time t_{BCM} given in Section 2.6.4. Thus, the estimate given in Ref. [7] shows this behavior.

In this BCM scenario, two conditions presented in Section 2.6.4 are the same except the change $t_{\text{BCM}} \rightarrow t_2$,

- The mass parameter should remain (almost) constant. The case for temperature-dependent mass is given recently [120].
- The commencement time of BCM is t_2 when the cosmic temperature is now denoted as T_2 .⁴

⁴Usually, the commencement time is expressed in terms of the corresponding cosmic temperature $T_1 = O(1 \text{ GeV})$. Certainly, T_2 is between T_1 and Λ_{QCD} , and the recent estimate [8] must be understood with this caveat.

6.1.2. Bose–Einstein condensation

In quantum mechanics with many particles, the ground-state level with $E = \frac{1}{2}\hbar\omega$ is filled by particles. In our case, the ground state is filled by bosonic particles. Being boson, the ground state of ϕ invites more bosons to be filled with the same quantum numbers, e.g., with the same momentum. This is the reason we call their motion *collective*. Even though the energy is split into potential and kinetic energies, their sum remains the same in the harmonic motion. Assuming that thermalization of the particles is achieved, this situation is shown in Fig. 6.3. In Fig. 6.3(a), higher levels are filled due to the temperature effect. At a sufficiently low temperature, most particles fill the ground state as shown in Fig. 6.3(b), which is the realization of the Bose–Einstein condensate. In this case, the particles in the ground state have the same momentum.

For the case of Fig. 6.1, the sum is the value of V at the bullet. This sum is the energy within the horizon. The horizon scale $R(t)$ expands, the energy inside the horizon remains the same (within the volume $\propto R(t)^3$), and hence our BCM behaves like CDM. In this case, BCM is the collective motion of Goldstone bosons with the same magnitude of momentum. So, the whole motion may be called collective motion. The BCM has the oscillation frequency m_0 , i.e., the vacuum value $\langle\phi\rangle$ oscillates with frequency m_0 . Bosons in the horizon have the same momentum. Because the BCM behaves like CDM, the ϕ particle momenta of BCM are negligible compared to mass m_0 and we can set it as zero in the homogeneous cosmic background. But our Galaxy and Sun moves with zero velocity in the homogeneous background, and hence the ϕ particle velocity can be taken as $-(\vec{v}_{\text{Galaxy}} + \vec{v}_{\text{Sun}})$, whose magnitude is usually taken as $\approx 220 \text{ km s}^{-1}$. If temperature is low enough, the dispersion due to the Boltzmann distribution is smaller than the dispersion due to the velocity of the measuring apparatus, which is practically of order 220 km s^{-1} .

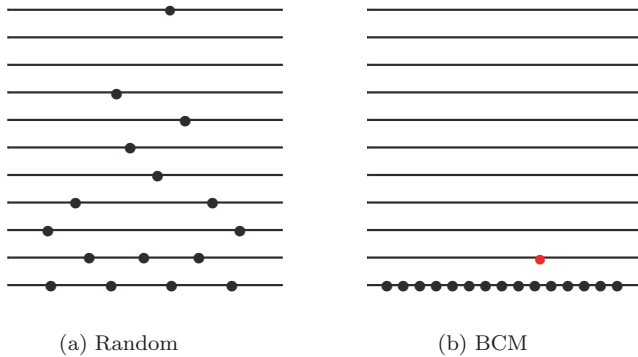


Fig. 6.3. Energy levels of harmonic oscillator: (a) Levels are filled randomly. (b) At very low temperature, most particles fill the ground states.

Classical limits

The classical limits are obtained by taking $\hbar \rightarrow 0$. But, there is a difference between the WIMP and BCM dark matters, in taking another limit:

$$\text{WIMP: } E = \hbar\omega = \text{fixed}, \quad \mathbf{p} = \hbar\mathbf{k} = \text{fixed}, \quad (6.25)$$

$$\text{BCM: } E = \mathcal{N}\hbar\omega = \text{fixed}, \quad \mathbf{p} = \mathcal{N}\hbar\mathbf{k} = \text{fixed}, \quad (6.26)$$

where $\mathcal{N}$ is the number of bosons which is related to the phase space number density by $\mathcal{N} = \hbar n_a$,

$$\begin{aligned} \mathcal{N} &= \frac{2\pi^3 n(t)}{\frac{4\pi}{3}(m_a \delta v)^3} \simeq 2 \cdot 10^{58} \left(\frac{f_a}{10^{11} \text{ GeV}} \right)^{8/3}, \\ \text{with } \delta v(t) &\simeq \frac{1}{m_a t_2} \frac{R(t_2)}{R(t)}. \end{aligned} \quad (6.27)$$

For the BCM case, viz. Eq. (6.26), $\hbar\omega$ is extremely small for a very large $\mathcal{N}$. In this case, we can proceed to discuss the Bose–Einstein condensation if another condition (thermalization condition) is satisfied. This difference of classical limits is stressed in [9], in relation to the caustic rings and the angular momenta of spiral galaxies.

Collective motion

The ground state corresponds to the bottom level of Fig. 6.3(b). But Goldstone bosons created by the vacuum motion are not necessarily at the ground state. For the Bose–Einstein condensation to be realized, “thermalization” has to be effective. Since the creation of QCD axions, thermalization has not occurred because thermalization requires statistical equilibrium. Creation of QCD axions by the $\langle a \rangle$ oscillation, by the condition $H = m_a/3$, during the QCD phase transition means that axions are not in the thermal equilibrium. At the creation time of axion quanta a_{quantum} , the axion vacuum $\langle a \rangle$ is at the red bullet of Fig. 6.1, with momentum of a_{quantum} vanishing. The number density n_a of a_{quantum} at the creation time is the required CDM energy density ρ_a which is the value V at the red bullet point, i.e., $\rho_a = n_a m_a$ with momentum $\mathbf{p}_a = 0$. When the axion vacuum rolls down the hill, the axion quanta obtain momenta which are not necessarily correlated. In this situation, axions are called in the collective motion. This phenomenon on axion vacuum applies to any BCM.

Coherent motion

For the BCM idea to be useful, the λ term plus $(\cdots)$ in Eq. (6.1) must be negligible. This is because the linearization must be effective for CDM ϕ . If the leading term

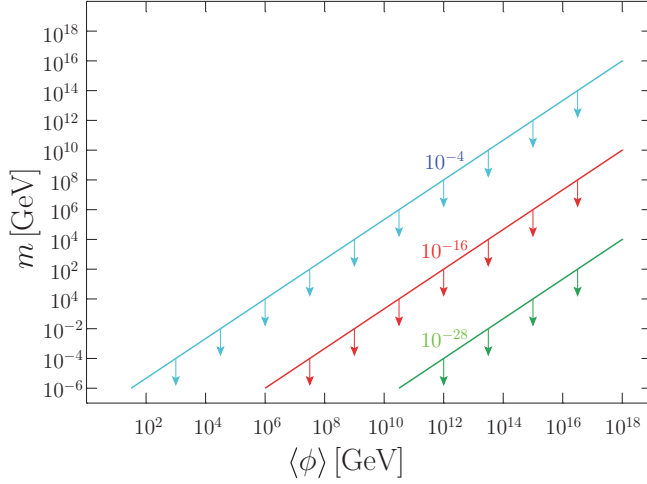


Fig. 6.4. The bound on λ is presented in the m vs. $\langle\phi\rangle$ plane. For a given set of m and $\langle\phi\rangle$, λ should be much less than the number given on the line.

among these is $\frac{\lambda}{4}\phi^4$, the BCM condition gives an inequality,

$$\lambda \ll \left(\frac{m}{\langle\phi\rangle} \right)^2. \quad (6.28)$$

It is sufficient to consider the leading term among interactions because we consider only scattering among quanta of axions. In Fig. 6.4, the above bound is presented in the m vs. $\langle\phi\rangle$ plane. For a given set of m and $\langle\phi\rangle$, λ should be much less than the number given on the line. For example, if $\langle\phi\rangle = 10^{12}$ GeV and $m = 10^4$ GeV, λ should be much less than 10^{-16} .

Below, we discuss the case of Goldstone bosons as BCM. Again, let us present the well-known QCD axion. To have a coherent motion, axion must be in thermal equilibrium such that uncorrelated $\mathbf{p}_a$ must find a reason to align at the vacuum. For an excited state of a_{quantum} in Fig. 6.3(a) to fall down to a ground state with a direction $\mathbf{p}_{a,0}$, with the energy difference given to some others, either by scattering by a quartic coupling $(\lambda/4)a^4$,

$$a_{\text{quantum}}(\mathbf{p}_1) + a_{\text{quantum}}(\mathbf{p}_2) \leftrightarrow a_{\text{quantum}}(\mathbf{p}_{a,0}) + a_{\text{quantum}}(\mathbf{p}_3), \quad (6.29)$$

or by radiation

$$a_{\text{quantum}}(\mathbf{p}_a) \rightarrow a_{\text{quantum}}(\mathbf{p}_{a,0}) + \text{radiation}. \quad (6.30)$$

As commented above, “radiation” in Eq. (6.30) cannot be electromagnetic waves. The process (6.30) for radiating gravitons is too small and can never be realized in our Universe.

The only remaining possibility (6.29) by gravitational interaction has been studied by Sikivie and Yang [10]. It may be possible because a_{quantum} in a gravitational

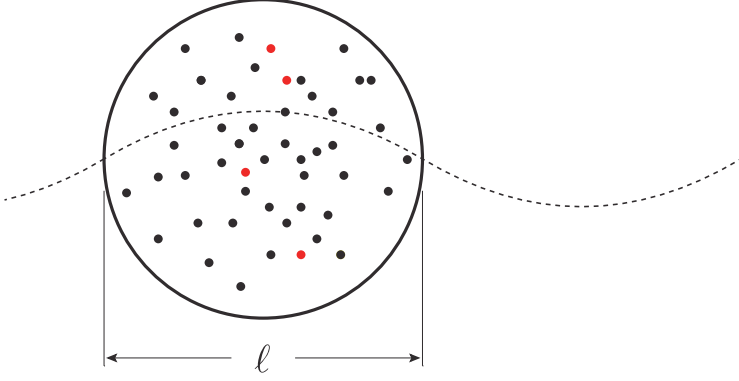


Fig. 6.5. A cosmological size $\ell < \ell_{\text{galaxy}}$ for low momentum axion. Some CDM axion quanta are shown as dots.

potential will experience force GMm_a/r^2 where r is the distance from the center of the potential and M is the mass inside the sphere of radius r . If so, a_{quantum} may go farther away spatially by processes (6.29), but with the final value of momenta as the ground state $\mathbf{p}_{a,0}$. This is the basis of “thermalization condition” by gravity. Here, two conditions have to be satisfied. Firstly, the energy difference between levels ω in Fig. 6.3 is small enough for any excited state to fall down by satisfying the energy conservation. It means that the corresponding wavelength is large enough to contain an enormous number of axions, N , within that scale, for example within the half wavelength in Fig. 6.5. Second, the epoch for the Bose–Einstein condensation has already happened, i.e., t_{BE} is shorter than the age of the Universe t_U . The total number of a_{quantum} in the ball of radius ℓ of Fig. 6.5 is

$$N = \frac{4\pi}{3} \ell^3 n_a^\ell. \quad (6.31)$$

Here, we consider ℓ a half of the de Broglie wavelength in Fig. 6.5.

When Γ_{int} is calculated with the phase space of $\sim T$ around the QCD phase transition, the decoupling temperature of order GeV is obtained at the time of QCD-phase transition [1, 7]. Below this temperature $T_{\text{dec}}^{\text{QCD}}$, axions behave like CDM as we will soon describe. But within some scale ℓ at a low temperature, the available phase space is $\mathbf{p}_a$ of Fig. 6.3 which is of order the velocity dispersion of the CDM axion. But the number in the volume ℓ^3 is enormous, and we can anticipate that axions can rethermalize at T_{dec}^ℓ of Fig. 6.6. This happens in the RD epoch by gravitational interaction, at $T \approx 500$ eV, as shown in Ref. [11].

Example 6.2 (Show that BEC is not possible for λa^4 interaction). Consider the $(\lambda/4)a^4$ interaction. The radiation–matter equality point occurs when the energy density of relativistic particles are $\nu_e, \bar{\nu}_e$, and photon, i.e., $g_* = 2|\gamma + 0.63|_\nu$,

$$H_{\text{eq}} \simeq 0.221 \cdot 10^{-24} T^2 \text{ keV}^{-1} \quad (\text{at the time of radiation} = \text{matter}). \quad (6.32)$$

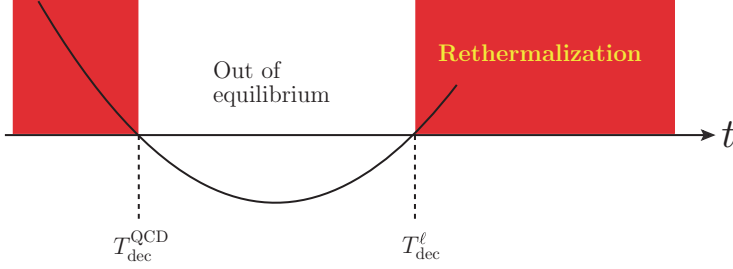


Fig. 6.6. Rethermalization at the scale ℓ . Between $T_{\text{dec}}^{\text{QCD}}$ and T_{dec}^{ℓ} axions are out of thermal equilibrium. The rethermalization by gravity occurred after T fell below 500 eV.

The needed matter density now is $\rho_{\text{matter}} = 0.33 \cdot 0.81 h^2 10^{-22} \text{ keV}^4$ which gives $\rho_{\text{eq}} = \rho_{\text{matter}}(t_{\text{U}}/t_{\text{eq}})^{3/2}$ at t_{eq} the time of radiation = matter. From t_{eq} , the density decreases as $t^{-3/2}$ (MD), and

$$\rho_{\text{eq}} = \left(\frac{t_{\text{U}}}{t_{\text{eq}}} \right)^{3/2} 0.33 \cdot 0.81 h^2 10^{-22} \text{ keV}^4 \quad (6.33)$$

$$= \left(\frac{T_{\text{eq}}}{2.72 \text{ K}} \right)^3 \cdot 0.33 \cdot 0.81 h^2 10^{-22} \text{ keV}^4 \quad (6.34)$$

$$= \left(\frac{T_{\text{eq}}}{2.34 \cdot 10^{-4} \text{ eV}} \right)^3 \cdot 0.33 \cdot 0.81 h^2 10^{-10} \text{ eV}^4 \quad (6.35)$$

$$= 9.646 \cdot 10^{-1} T_{\text{eq}}^3 \text{ eV}. \quad (6.36)$$

The energy density from (6.32) is

$$\rho_{\text{eq}} = 3M_{\text{P}}^2 H_{\text{eq}}^2 = 3 \cdot (2.43^2)(0.221^2) T_{\text{eq}}^4. \quad (6.37)$$

Comparing (6.36) and (6.37), the temperature at the time of radiation = matter is, for $h \simeq 0.68$,⁵

$$T_{\text{eq}} \simeq 0.755 \text{ eV}, \quad \text{and} \quad \rho_{\text{eq}} \simeq 0.287 \text{ eV}^4. \quad (6.38)$$

Then, at a lower temperature $T_{\ell} < T_{\text{eq}}$, the number density of axions is, if CDM is composed of QCD axions only,

$$\begin{aligned} n_a^{\ell} &= \left(\frac{\rho_{\text{eq}}}{m_a} \right) \left(\frac{T_{\text{eq}}}{T_{\ell}} \right)^3 \simeq \frac{0.287 \text{ eV}^4 f_a}{0.61 \cdot 10^{16} \text{ eV}} \left(\frac{T_{\text{eq}}}{T_{\ell}} \right)^3 \\ &\simeq 1.02 \cdot 10^4 \left(\frac{f_a}{10^{11} \text{ GeV}} \right) \left(\frac{T_{\text{eq}}}{T_{\ell}} \right)^3 \text{ eV}^4. \end{aligned} \quad (6.39)$$

⁵The Planck data gives $z_{\text{eq}} = 3382 \pm 32$ [13].

The scattering cross-section for (6.29) is of order

$$\sigma \sim \frac{\lambda^2}{32\pi} \frac{1}{m_a^2} \simeq \frac{\Lambda^4}{256\pi f_a^4} \frac{1}{m_a^2} \simeq \frac{1}{128\pi f_a^2}, \quad (6.40)$$

where we used m_a vs. f_a relation of Section 6.3. Even though the rate $\langle\sigma v\rangle$ due to cross-section is so small, the final ground-state number N can be astronomical such that Bose–Einstein enhancement of the transition probability has occurred. Note that the process (6.29) has amplitudes proportional to $\sqrt{N+1}$ for the forward direction and $\sqrt{N}$ for the backward direction [12].⁶ These are practically equal and the ground state achieves thermal equilibrium. This resetting of thermal equilibrium of axion is possible if $\langle\sigma v\rangle N\ell^{-3} \gg H \sim \ell^{-1}$, for a sub-galaxy size ℓ ,

$$\left(\frac{10^{-4}}{128\pi f_a^2}\right) \frac{4\pi}{3} \ell^{-3} \gg \frac{4\pi}{3} \ell^3 \cdot 1.02 \cdot 10^4 \left(\frac{f_a}{10^{11} \text{ GeV}}\right) \left(\frac{T_{\text{eq}}}{T_\ell}\right)^3 \text{ eV}^4. \quad (6.41)$$

It is not possible because

$$\left(\frac{\ell^{-1}}{\text{eV}}\right)^6 \gg 4.1 \cdot 10^{50} \left(\frac{T_{\text{eq}}}{T_\ell}\right)^3 \left(\frac{f_a}{10^{11} \text{ GeV}}\right)^3 \quad (6.42)$$

cannot be satisfied in the region below 270 MeV scale for ℓ^{-1} .

However, considering gravity, it has been shown that the Bose–Einstein condensation has occurred, and axion quanta entered into “thermal equilibrium”, behaving as a coherent motion with the same $\mathbf{p}_{a,0}$ by gravitational interaction. It occurred at the photon temperature [11]

$$T_\gamma^{\text{BEC}} \approx 170 x \left(\frac{f_a}{10^{11} \text{ GeV}}\right)^{1/2} [\text{eV}], \quad (6.43)$$

where x is the energy increase factor by the decay of axion strings [14–16]. This is a special case for the QCD axion where we used the relation between mass and decay constant of Section 6.3.

Bose–Einstein condensation in cosmology has also been considered for an ultra-light boson with mass in the range 10^{-22} eV [17–20]. An interesting possibility from the symmetry principle is given for an ultra-light axion (ULA) [21, 22]. The Compton wavelength (not the de Broglie wavelength considered for the QCD axion) of these ULAs encompass a sub-galaxy scales, which was used to solve the cusp-core problem. So, the picture in these ULAs is not the one depicted in Fig. 6.5 because the particles cannot be located in that way, but a collection of waves must be pictured overlapping each other within ℓ .

⁶A detail expression is given in Ref. [11].

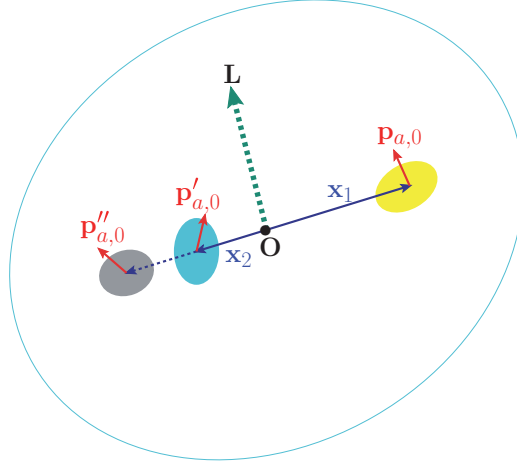


Fig. 6.7. Creation of galactic angular momentum $\mathbf{L}$. At different regions of correlated Bose–Einstein gas, the ground-state momenta are different $\mathbf{p}_{a,0}, \mathbf{p}'_{a,0}, \mathbf{p}''_{a,0}$, etc. If there is a huge mass center, probably outside the galaxy, then a galactic momentum $\mathbf{L}$ can be present.

6.1.3. Galactic angular momentum by BCM

If the axion quanta are rethermalized, we can visualize the situation within a galaxy as shown in Fig. 6.7. Let the center of a galaxy is defined to be at $\mathbf{x}_{\text{CM}} = 0$ such that

$$\sum_i m_i \mathbf{x}_i = 0, \quad \sum_i m_i = M. \quad (6.44)$$

The mini-halo sizes are all different with different ground-state momenta, because ℓ of Fig. 6.5 is smaller than the galactic scale. The Bose–Einstein condensed particles have the same momentum, $\mathbf{p}_{a,0}$, within one correlated Bose–Einstein gas, but the ground-state momenta will be different at different regions of Bose–Einstein gas, as shown in Fig. 6.7. In addition, their sizes and shapes are different at different correlation regions.

From a distance ℓ , the angular momentum of a sub-halo is $m|\mathbf{v}|/\mathcal{N} \times \mathcal{N} \times \ell \approx m|\mathbf{v}|\ell$ where $\mathcal{N}$ is the occupation number of CDM axion. If it rotates in the galaxy with frequency ω , we estimate it as $M\ell^2\omega \approx M|\mathbf{v}|\ell$. With the uniform velocity $|\mathbf{v}| = O(300 \text{ km/s})$ at a remote position of a galactic arm $\ell = O(30 \text{ kpc})$, frequency is of order $\omega = O(10^{-13})$. Having this order of $|\mathbf{p}_{a,0}|$ in Eq. (6.29) is a random choice. For such a choice, an orbital angular momentum is generated. Thus, there will result a nonvanishing orbital angular momentum of a galaxy, presumably explaining some portion of galactic angular momentum. Of course, the scattering processes conserve the total angular momentum, and it looks like an angular momentum cannot be generated. But, the angular momentum shown by galactic arms is just an orbital

angular momentum. So, if nucleons participate in the thermalization process, nucleons may carry away some angular momentum. So, some orbital angular momentum can be generated. It will be interesting if this idea can be checked experimentally. For the ULA with mass 10^{-22} eV, this explanation of orbital angular momentum does not apply because the ULA has not gone to the Bose–Einstein condensation state.

If the velocity field of axion gas is rotational, there can be caustic rings [23]. The axion condensation that rethermalizes quickly was used for explaining the caustic rings for ℓ larger than the galactic scale.

Example 6.3 (Effective inertia of rotation). Suppose that a mass shell of thickness dx at x from the origin $\mathbf{O}$ has rotational inertia $dI = A\rho(x)4\pi x^4 dx = Ax^2 dm$ with $dm = \rho(x)4\pi x^2 dx$. With the density profile, the effective inertia of rotation is

$$\begin{aligned} I_{\text{eff}} &= A \int_{R_s}^{R_{\text{max}}} \rho(x) 4\pi x^4 dx = 4\pi A \int_1^{\xi_m} \frac{\rho_0 R_s^5}{[1 + \xi]^2} \xi^3 d\xi \\ &= 2\pi A \rho_0 R_s^3 R_{\text{max}}^2 \left[1 - 4\xi_m^{-1} + 3\xi_m^{-2} + 6\xi_m^{-2} \ln(1 + \xi_m) \right. \\ &\quad \left. - 6\xi_m^{-2} \ln 2 - \xi_m^{-2} \frac{\xi_m - 1}{\xi_m + 1} \right] \approx 2\pi A \rho_0 R_s^3 R_{\text{max}}^2, \end{aligned} \quad (6.45)$$

where $A = 2/3$ for a spherical shell. The Navarro–Frenk–White profile [24] is

$$\rho(r) = \frac{\rho_0}{\frac{r}{R_s} [1 + (r/R_s)]^2} \quad (6.46)$$

with

$$M = 4\pi \rho_0 R_s^3 \left[\ln(1 + \xi_m) - \frac{\xi_m}{1 + \xi_m} \right]. \quad (6.47)$$

Even though the total mass, obtained by integrating to ∞ , is divergent, we can take the size as R_{max} . The value $R_{\text{max}}/R_s = \xi_m$ is between 15 and 20 for the Milky Way. Taking $\xi_m = 17.5$, we have $M \simeq 8\pi \rho_0 R_s^3$ and $I_{\text{eff}} \approx \frac{1}{6} M R_{\text{max}}^2$.

6.2. Scalars and pseudoscalars

For a boson to be CDM, the condition that its mass is comparable to the Hubble expansion rate at some late time, $m \simeq 3H$, hints that the boson (being very light) is better to be a kind of Goldstone boson. Thus, spontaneous symmetry breaking of some global U(1) is suitable for this purpose. Global symmetries are always broken with the gravity included as discussed in Chapter 4 and Section 6.6. Thus, mass m is nonzero, but its magnitude depends on the magnitude of the explicit breaking terms of the global symmetry. In an ultraviolet completed theory, popular high energy scales are M_{P} , M_{GUT} , and possibly an intermediate scale M_{int} . Depending

on the parity eigenvalue P , the Goldstone boson is called “scalar” for $P = +$ or “pseudoscalar” for $P = -$. It is usually given by the couplings to matter, i.e., depends on the couplings to fermions. A scalar s couples to a Dirac fermion ψ as $\bar{\psi}\psi s$, and a pseudoscalar a couples as $\bar{\psi}i\gamma_5\psi a$.

For a pseudoscalar Goldstone boson, it can be represented as a phase field of the complex spin-0 field Φ , viz. Section 4.4,

$$\Phi = \frac{f + \rho}{\sqrt{2}} e^{ia/f}, \quad (6.48)$$

where $\langle\Phi\rangle = f/\sqrt{2}$ and ρ is the radial field with the vacuum value $\langle\rho\rangle = 0$. Definition of the pseudoscalar Goldstone boson by (6.48) makes sense since it accompanies the $U(1)$ symmetry breaking scale f . Then, the leading coupling of a to fermion ψ is proportional to

$$\bar{\psi}_R\psi_L f e^{ia/f} + \text{h.c.} = \bar{\psi}i\gamma_5\psi a, \quad (6.49)$$

which is the desired form. The phase field corresponds to the rotation angle α of the global $U(1)$ symmetry, $a \rightarrow a + f\alpha$.

A scalar field can be made to couple to fermions, at least by gravitational interaction even if its fermion coupling is declared to be zero in the beginning. As shown in Eqs. (6.48) and (6.49), a scalar Goldstone boson s cannot be a phase field. The way it is realized is nonlinear as discussed in Section 4.4,

$$s \rightarrow s + \text{constant}, \quad (6.50)$$

which can be exponentiated as

$$S = \Lambda e^{s/f_s}. \quad (6.51)$$

Thus, a shift of s along Eq. (6.51) actually changes the scale Λ , and the scalar s is “dilaton” or “scale-Goldstone boson”. The symmetry (6.51) is “dilatic” symmetry or “scale” symmetry.

Massive pseudoscalar boson as phase field

If we consider loop corrections without any vertices violating the global $U(1)$ symmetry, the phase (pseudoscalar) field a does not appear in the loop integral. A typical contribution is shown in Fig. 6.8. At each vertex, there do not appear phase fields, and the whole diagram satisfies the global $U(1)$ symmetry. The vacuum energy is contributed by diagrams with no external lines.

A scalar field s does not enjoy this simple diagrammatic explanation, because the related invariance is a (real) gauge transformation e^α instead of a phase transformation $e^{i\alpha}$. Therefore, these loop diagrams do not satisfy the real gauge transformation automatically. For example, the contribution to the cosmological constant (CC) is by diagrams with no external lines. These do not respect the (real) gauge

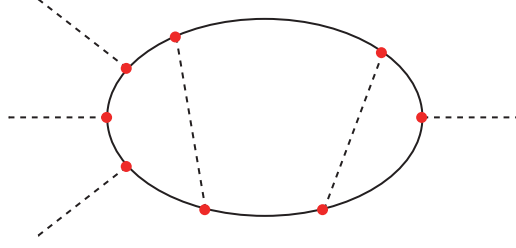


Fig. 6.8. A loop correction to a potential term of Φ . The vacuum energy is contributed by diagrams with no external lines. At the vertices, the phase field a does not appear and the whole diagram satisfies the global $U(1)$ symmetry.

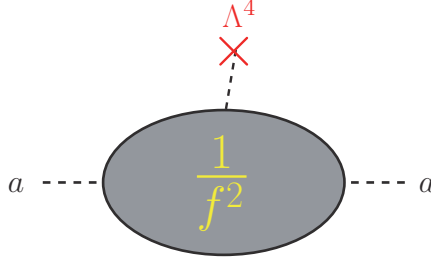


Fig. 6.9. A mass diagram for a pseudoscalar Goldstone boson a .

transformation⁷ even if all vertices (with only dimension 4 couplings) satisfy the (real) gauge transformation. To obtain a vanishing contribution from the scalar boson, one must invoke an extra symmetry beyond the (real) gauge transformation.

The (Goldstone) phase field does not appear in the potential if the corresponding $U(1)$ symmetry is not explicitly broken. If the $U(1)$ symmetry is explicitly broken, the Goldstone boson obtains mass by the insertion of the explicit symmetry breaking term in the diagrams of the type shown in Fig. 6.9. Thus, the mass term from Fig. 6.9 is (coupling constants) $\times \Lambda^4/f^2$, with two external pseudoscalar lines. This term belongs to the red part in Fig. 4.5. For a pseudoscalar Goldstone boson, therefore, we can study the explicit breaking terms more concretely in a top-down approach. For simplicity, we consider only one complex field Φ , carrying the $U(1)$ charge, and write the explicit symmetry breaking term as

$$V_{\text{viol}} = \sum_n \frac{c_n}{2M^{n-4}} \Phi^n + \text{h.c.} = \sum_n \frac{|c_n|}{M^{n-4}} \cos\left(\frac{na}{f} + \delta_n\right), \quad (6.52)$$

where $c_n = |c_n|e^{i\delta_n}$ and M is a cutoff scale. We require n start from 5 so that the breaking term is small at the scale M . Because of this periodic form, higher

⁷For the dilaton symmetry, we need dimension 4 coupling, i.e., $s^4 \rightarrow e^{4\alpha} s^4$ under the transformation.

order terms can satisfy the BCM condition suggested in Eq. (2.90). Usually, some discrete symmetries can achieve this in the top-down approach [25]. Many GUT scale pseudoscalars such as in the N -flation scenario [26] employ this kind of potential.

6.3. Axions

There is an important case that only one coupling constant is present in Eq. (6.52), which can be compared to the successful case of one coupling constant G_F (by the “V–A” theory) out of 34 couplings in Fermi’s β -decay Hamiltonian, as discussed in the beginning of Chapter 4.

6.3.1. Emergence of axion as BCM

This important case is realized when the global $U(1)$ is broken by a non-Abelian gauge group anomaly, i.e., there exists the $U(1)_{\text{global}} \times G^2$ non-Abelian anomaly where G is a non-Abelian gauge group. Only one $U(1)_{\text{global}}$ breaking term, i.e., only one coupling, is possible here because the Adler–Bell–Jackiw anomaly [27] is described only by oneloop. Higher order corrections do not introduce any new type of anomaly [28]. This explicit breaking of $U(1)_{\text{global}}$ by non-Abelian anomaly was applied to the strong CP problem [29]. In this case, the $U(1)_{\text{global}}$ is called the “Peccei–Quinn (PQ) symmetry”, $U(1)_{\text{PQ}}$. Below the scale of PQ symmetry breaking, the resulting Goldstone boson is called *axion* and f is called the *axion decay constant* f_a . In a historical order, below we discuss how the axion as BCM was realized.

The $U(1)$ problem

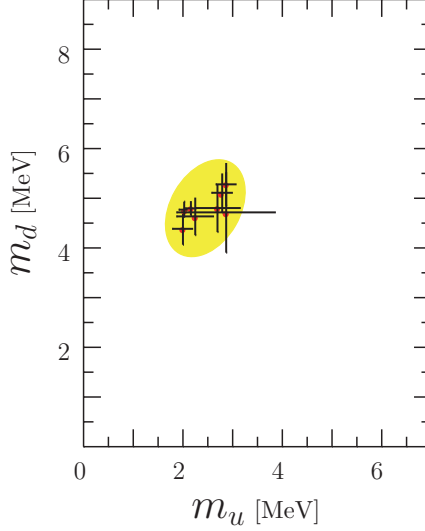
The modern theory of strong interaction QCD is the $SU(3)$ gauge theory with the light quark masses as inputs at the QCD scale around several hundred MeV,

$$\mathcal{L}_{\text{mass}} = -m_u \bar{u}_R u_L - m_d \bar{d}_R d_L - m_s \bar{s}_R s_L + \text{h.c.} \quad (6.53)$$

The current limit on the light quark masses are $O(5 \text{ MeV})$ for m_u and m_d as shown in Fig. 6.10 [30], and m_s is about 20 times m_d . Since the lightest quark u has nonzero mass near 2.5 MeV, there is no quark with zero mass [30]. This means that the chiral symmetry $\psi \rightarrow e^{i\alpha\gamma_5} \psi$ is explicitly broken by the above QCD mass terms because $\psi_{L,R}$ transform as

$$\psi_L \rightarrow e^{i\alpha} \psi_L, \quad \bar{\psi}_L = \bar{\psi} e^{-i\alpha}, \quad (6.54)$$

$$\psi_R \rightarrow e^{-i\alpha} \psi_R, \quad \bar{\psi}_R \rightarrow \bar{\psi} e^{i\alpha}, \quad (6.55)$$


 Fig. 6.10. The mass bounds of u and d quarks [30].

where we used the notation

$$\psi_L = \frac{1+\gamma_5}{2} \psi, \quad \bar{\psi}_L = \bar{\psi} \frac{1-\gamma_5}{2}, \quad (6.56)$$

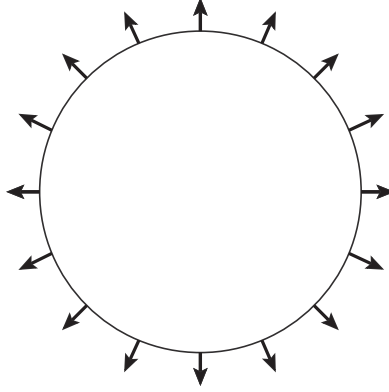
$$\psi_R = \frac{1-\gamma_5}{2} \psi, \quad \bar{\psi}_R = \bar{\psi} \frac{1+\gamma_5}{2}. \quad (6.57)$$

From Eq. (6.53), we note that QCD has the chiral symmetry in the limit $m_u, m_d, m_s \rightarrow 0$. The chiral symmetry with u and d quarks is $U(2)$,⁸

$$\begin{pmatrix} u \\ d \end{pmatrix} \rightarrow e^{i\alpha^a F^a \gamma_5} \begin{pmatrix} u \\ d \end{pmatrix}, \quad (6.58)$$

where F^a ($a = 1, \dots, 4$) are 2×2 Hermitian matrices. Among these, the traceless matrices are three generators of $SU(2)$, $\frac{1}{2}\sigma^x$, $\frac{1}{2}\sigma^y$, $\frac{1}{2}\sigma^z$, and the other is 2×2 identity, $\frac{1}{2}\mathbf{1}$. When the chiral symmetry is exact at the Lagrangian level but is broken in the vacuum, there appear four Goldstone bosons. But, the chiral symmetry is broken by tiny amount by quark masses as discussed above, even though they are small compared to the strong interaction scale of order 1 GeV. So, these four Goldstone bosons are in fact pseudo-Goldstone bosons with mass $\propto (\text{quark mass} \times \Lambda_{\text{QCD}}^3)^{1/4}$. Indeed, three pion masses are very small, viz. $(0.14 \text{ GeV})^2 \ll 1 \text{ GeV}^2$. Except these three pseudo-Goldstone bosons, there is the fourth pseudo-Goldstone boson whose

⁸We can generalize to 3×3 , but the essence is here with two quarks.

Fig. 6.11. The hedgehog configuration of $\mathbf{A}$.

mass is estimated as [31]

$$m_{\eta'} \leq \sqrt{3} m_{\pi}. \quad (6.59)$$

The lightest SU(3) singlet⁹ pseudo-Goldstone is η' whose mass squared is 0.918 GeV^2 which is much larger than $3m_{\pi^+}^2 \simeq 0.02 \text{ GeV}^2$, violating the bound (6.59). Thus, the QCD has the η' mass problem which is called the “U(1) problem”.

The $\bar{\theta}$ -vacuum

Non-Abelian gauge theories have instanton solutions [32]. Let us present the case in the Euclidian space with metric $\eta_{\mu\nu}^{\text{Eucl}} = \text{diag}(+1, +1, +1, +1)$. At the radial infinity, the gauge field values of gauge group G need not vanish by identifying the radial direction of an SU(2) gauge field $\mathbf{A}$ to the radial direction of the Euclidian space as shown in Fig. 6.11. One can always choose a subgroup of G as the SU(2), and hence the following discussion applies to any non-Abelian gauge theories. The field configuration gives an integer called the *Pontryagin index*,

$$n = \frac{1}{32\pi^2} \int d^3x F_{\mu\nu}^i \tilde{F}^{i\mu\nu}, \quad (6.60)$$

where $F_{\mu\nu}^i$ is the field strength of $\mathbf{A}$ and $\tilde{F}^{i\mu\nu}$ is its dual, $\tilde{F}^{i\mu\nu} = \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} F_{\rho\sigma}^i$. The vacuum of gauge field $\mathbf{A}$ is called the n -vacuum. Since the n -vacuum $|n\rangle$ of (6.60)

⁹With three quarks, we obtain the bound on the lightest SU(3) singlet meson η' .

is not gauge invariant, one defines the gauge invariant vacuum, $|\theta\rangle$,

$$|\theta\rangle = \sum_{n=-\infty}^{+\infty} e^{i n \theta} |n\rangle \quad (6.61)$$

which is called the θ -vacuum. In the θ -vacuum, there exists a free energy term [33],

$$V_{\text{vac}} = \frac{\theta}{32\pi^2} F_{\mu\nu}^i \tilde{F}^{i\mu\nu} \equiv \theta \{F\tilde{F}\}. \quad (6.62)$$

A relevant question is: “Is the θ parameter of (6.62) physical?” It is widely accepted that it is. The most convincing argument for the physical significance of (6.62) is related to the solution of the U(1) problem of QCD. The U(1) problem is understood by introducing the above effective Lagrangian derived in the θ -vacuum. The shift of the η' field by $f_{\eta'}\alpha$, $\eta' \rightarrow \eta' + \alpha f_{\eta'}$, is equivalent to introducing a term $\alpha\{F\tilde{F}\}$ of Eq. (6.62), i.e., $(\eta'/f_{\eta'})\{F\tilde{F}\}$, namely, η' couples to gluons directly, in addition to the small effect of (6.59) via light quarks and obtains mass close to the strong interaction scale of 1 GeV. So, the θ -vacuum solves the U(1) problem [34]. This is the best solution of the U(1) problem, and we consider the term $\theta\{F\tilde{F}\}$ physical.

The strong CP problem

The strong CP problem starts from the observed upper bound on the neutron electric dipole moment (NEDM). If the theory of strong interactions violates the CP symmetry at a full strength, a natural value of NEDM d_n is expected to be (charge) $\times$ (radius) of neutron, i.e., $O(10^{-13} \text{ e cm})$. But, the current lower bound on NEDM is [35]

$$|d_n| < 2.9 \times 10^{-26} \text{ e cm (90\% CL)}. \quad (6.63)$$

Consider Eq. (6.62) in terms of the gluon field strength. Suppose that Eq. (6.52) is the only term violating CP at the strong interaction scale. Then, Eq. (6.52) implies that the coefficient of CP violating term at the strong interaction scale is much less than $\lesssim 10^{-13}$. Thus, we face a fine-tuning problem that the coefficient θ should be tuned to $\lesssim 10^{-13}$, raised to $O(10^{-10})$ due to the coefficient in Eq. (6.62).

Since θ of Eq. (6.62) is a physical parameter, the bound (6.63) gives a bound on the θ parameter, including the electroweak CP violation effect,

$$|\bar{\theta}| = |\theta + \text{argument of Det } M_q|, \quad (6.64)$$

where M_q is the quark mass matrix. We will present the above form of the observable $|\bar{\theta}|$ shortly. On the other hand, with the interaction (6.62), we expect [36, 37]

$$d_n(|\bar{\theta}|) \simeq \begin{cases} |\bar{\theta}| \frac{m_*}{\Lambda_{\text{QCD}}} \frac{e}{m_n} \left[\text{with } m_* = \frac{m_u m_d}{m_u + m_d} \right] \approx |\bar{\theta}| \cdot (6 \times 10^{-16}) e \text{ cm}, \\ |\bar{\theta}| \frac{g_{\pi nn}}{12\pi^2} \frac{e}{m_n} \ln \left(\frac{m_n}{m_{\pi^0}} \right) \approx |\bar{\theta}| \cdot (4.5 \times 10^{-15}) e \text{ cm}, \end{cases} \quad (6.65)$$

from which we have $|\bar{\theta}| < 10^{-10} - 10^{-11}$. “Why is $\bar{\theta}$ so small?” is the *strong CP problem*.

Need for a theory of weak CP violation

The weak CP violation has been discovered in a K meson decay in 1964 [38] and also confirmed in the B meson decays in 2002 [39]. Right after the discovery, the tiny strength of weak CP violation was a mystery as symbolized by the phrase of “very weak interaction” [40]. After the advent of gauge theories, quark models were used first by Mohapatra with a right-handed current [41], but now the experimentally confirmed theory is the Kobayashi–Maskawa (KM) model based on three families [42]. The Mohapatra model uses three chiral doublets, but has the flavor changing neutral current problem among right-handed currents [42], and one can view the KM model as using three left-handed chiral doublets. In retrospect, Mohapatra’s RH doublet could be made a LH doublet to be free from the flavor-changing neutral current problem. [Of course, that LH doublet should be beyond the already introduced two LH doublets.] The origin of the so-called CKM matrix is through complex Yukawa couplings and hence through the complex mass matrix as discussed in Chapter 4. The diagonalization process of the complex mass matrix employs the bi-unitary transformation, both on the left-handed quarks and on the right-handed quarks. The unitary transformation, $\psi \rightarrow e^{i\alpha}\psi$, does not change the chirality. But the chiral transformation, $\psi \rightarrow e^{i\alpha\gamma_5}\psi$, changes chirality, as explicitly shown in Eqs. (6.54) and (6.55). This chiral transformation introduces the anomaly term

$$\frac{2\alpha}{32\pi^2} G_{\mu\nu}^a \tilde{G}^{a\mu\nu}, \quad (6.66)$$

where $G_{\mu\nu}^a$ is the field strength of gluon field A_μ^a . Thus, the final vacuum angle is changed and the resultant one is the experimentally measurable $\bar{\theta}$ of Eq. (6.64).

There are five possible methods to introduce the weak CP violation, including the three examples of Ref. [42]:

- (1) by light-colored scalar,
- (2) by right-handed current(s),
- (3) by three left-handed families, (6.67)
- (4) by propagators of light color-singlet scalars, and
- (5) by an extra U(1) gauge interaction.

The first three are those of Ref. [42], among which the second was presented in Ref. [41] also, and the fourth and the fifth are not listed there. Item (3) is the so-called KM model, leading to the current CKM matrix. Item (4) is the Weinberg model if Higgs doublets are involved [43] or a kind of superweak model with $SU(2)_L$ singlet scalars. Item (5) can be considered as a kind of superweak model with an extra gauge interaction.

Potential with many Higgs doublets

If the quark families were only two, the weak CP violation must come from a sector which does not involve quarks. In the SM, no right-handed charged current is allowed. Barring light colored scalars due to the fact that no unexpected hadrons below a few hundred GeV has been observed, the only possibility in this case is item (4) in (6.67). Then, the weak CP violation must come from the Higgs potential with multi-Higgs doublets [43],

$$V_W = -\frac{1}{2} \sum_I m_I^2 \phi_I^\dagger \phi_I + \frac{1}{4} \sum_{IJ} [a_{IJ} \phi_I^\dagger \phi_I \phi_J^\dagger \phi_J + b_{IJ} \phi_I^\dagger \phi_J \phi_J^\dagger \phi_I + c_{IJ} \phi_I^\dagger \phi_J \phi_I^\dagger \phi_J] + \text{h.c.}, \quad (6.68)$$

where the reflection symmetry $\phi_I \rightarrow -\phi_I$ is imposed. The mass parameters m_I^2 are at the electroweak scale such that the electroweak symmetry is broken at the electroweak scale. With the potential (6.68), three Higgs doublets are needed to introduce CP violation [43]. Not to introduce flavor changing neutral currents, Ref. [43] required that only one Higgs doublet, ϕ_1 , couples to $Q_{\text{em}} = \frac{2}{3}$ quarks, and another Higgs doublet, ϕ_2 , couples to $Q_{\text{em}} = -\frac{1}{3}$ quarks [44]. The reflection symmetries, including nontrivial transformations of the quark fields, will achieve this goal. For all scalars and pseudoscalars of ϕ_I to obtain mass, all parameters in (6.68) are required to be nonzero.

Peccei–Quinn symmetry

Peccei and Quinn observed that if all c_{IJ} in Eq. (6.68) are zero, then the discrete symmetry is promoted to a global symmetry which we now call the PQ symmetry,

$$q_L \rightarrow q_L, \quad (6.69)$$

$$u_R \rightarrow e^{-i\alpha} u_R, \quad (6.70)$$

$$d_R \rightarrow e^{-i\beta} d_R, \quad (6.71)$$

$$\phi_1 \rightarrow e^{i\alpha} \phi_1, \quad (6.72)$$

$$\phi_2 \rightarrow e^{i\beta} \phi_2, \quad (6.73)$$

where q_L 's are the left-handed quark doublets, u_R 's are the right-handed up-type quark singlets, and d_R 's are the right-handed down-type quark singlets. Quarks obtain masses by

$$-\bar{q}_L u_R \phi_1 - \bar{q}_L d_R \phi_2 + \text{h.c.} \quad (6.74)$$

This PQ transformation is a chiral transformation, Eqs. (6.70) and (6.71), creating the anomaly coefficient of (6.66). Therefore, this simple phase transformation is thought to be equivalent to the gluon anomaly and in any physical processes, therefore, the phase will not appear and there is no strong CP problem.

Electroweak scale axion

The above PQ symmetry (if exact) must lead to an exactly massless Goldstone boson because quarks must obtain masses by the vacuum expectation values (VEVs) of ϕ_1 and ϕ_2 , i.e., the PQ symmetry must be spontaneously broken. However, the PQ symmetry is explicitly broken at quantum level because the QCD anomaly is present. Thus, the Goldstone boson becomes a pseudo-Goldstone boson, obtaining mass of order $\Lambda_{\text{QCD}}^2/v_{\text{ew}}$ by our general argument. This pseudo-Goldstone boson was named *axion*. From V_W of Eq. (6.68), we can separate out this axion direction. If c_{12} were present, which signifies the breaking of the PQ symmetry, the phase $e^{-i(a_1/v_1 - a_2/v_2)}$ will appear. Thus, the axion direction is

$$a \propto \frac{a_u}{v_u} - \frac{a_d}{v_d}, \quad (6.75)$$

where $\langle \phi_1 \rangle = (v_u + \rho_1)e^{ia_u/v_u}/\sqrt{2}$ and $\langle \phi_2 \rangle = (v_d + \rho_2)e^{ia_d/v_d}/\sqrt{2}$. This electroweak scale axion is called the Peccei–Quinn–Weinberg–Wilczek (PQWW) axion, having mass ~ 100 keV and lifetime $\sim$ second order [45–47].

Possibilities for small $\bar{\theta}$

The PQWW axion was not discovered [48], which has led to ideas on models without the PQWW axion. These are called “natural solutions” or “calculable solutions”. It is based on a symmetry which is realized in the limit $\bar{\theta} \rightarrow 0$. The symmetry realized in the limit $\bar{\theta} \rightarrow 0$ is CP. So, the whole Lagrangian is declared to be CP invariant in natural type solutions, which means effectively that all Yukawa couplings are real. It does not belong to item (3) in Eq. (6.67). The essence of CP violation in this case is spontaneous CP violation [49] and furthermore belongs to item (5) of Eq. (6.67), Ref. [50] for an extra U(1) and items (2) and (5) of Eq. (6.67), Ref. [51] for an extra SU(2)_R, Ref. [52] only with spontaneous CP violation [49] with an S_3 discrete symmetry, and Ref. [53] for item (5) for a superweak CP violation of Eq. (6.67). These can be called natural models with extra gauge interactions. Also, the case of soft CP violation with complex mass parameters of multi-Higgs doublets, not belonging to the spontaneous CP violation, belongs to item (4) of Eq. (6.67) [54].

This last case simply imposes the CP invariance for renormalizable couplings, but allows complex scalar mass parameters, and it is better called a calculable model with an initial $\bar{\theta} = 0$.

Firstly, all these models have to show that loop corrections do not lead to $|\bar{\theta}_{\text{by loops}}| > 10^{-10}$. Usually, one loop correction offers $\bar{\theta}$ of order $10^{-3}\alpha$ [50]. Second, successes of the suggested solutions depend on the possibility of explaining the observed CP violation phenomena. Since the confirmed CP violation theory [30] is item (3) in Eq. (6.67), the early calculable models are ruled out. The natural models suggested later by Nelson and Barr [55] is item (4) in Eq. (6.67) with color singlet *scalars*, allowing complex VEVs, such that at low energy, the Higgs doublet couplings are effectively considered to be complex [56]. In this class of the Nelson–Barr type solutions, one has to show $|\bar{\theta}_{\text{by loops}}| < 10^{-10}$, which is difficult to be realistically fulfilled [37].

Invisible axion

Because of the difficulties faced in the PQWW axion and calculable models, the PQ symmetry is reintroduced such that it is broken at a high energy scale. Not to interrupt the electroweak scale phenomenology, firstly the hypothetical axion is housed in an SU(2) singlet [2]. Furthermore, the color anomaly is needed. With the color anomaly, it was shown that $\bar{\theta} = 0$ is the minimum of free energy [57], and the cosmic vacuum chooses $\bar{\theta} = 0$ in the end of its evolution.

In simple models, the color anomaly can be introduced by the PQ charges of a heavy quark [2, 3] or by the PQ charges of light quarks [4, 5]. Since the axion appears as the phase of the singlet σ [2], the heavy quark Q coupling can be

$$-f_{QQ\sigma}\bar{Q}_L Q_R \sigma + \text{h.c.}, \quad (6.76)$$

which is called the Kim–Shifman–Vainstein–Zakharov (KSVZ) model. A low energy effective theory, after integrating out heavy fields, is described by the anomaly coupling

$$\text{KSVZ:}\mathcal{L}_{\text{int}} = \frac{g_c^2 a}{32\pi^2 f_a} G_{\mu\nu}^a \tilde{G}^{a\mu\nu}, \quad (6.77)$$

where $\tilde{G}^{a\mu\nu} = \frac{1}{2}\epsilon^{a\mu\nu\rho\sigma}G_{\rho\sigma}$.

To provide the color anomaly by light quarks, one has to couple σ , housing the axion, to light quarks, which led to the Dine–Fischler–Srednicki–Zhitnitsky (DFSZ) axions. But there is no renormalizable couplings of σ to q, u^c , and d^c due to the electroweak gauge symmetry. The definition of the PQ charge of σ is through coupling

to the up-type Higgs $H_u = \phi_1$ and the down-type Higgs $H_d = \phi_2$,

$$\text{DFSZ: } V = \begin{cases} \lambda \sigma^2 H_u H_d + \text{h.c.}, \\ \text{or} \\ M \sigma H_u H_d + \text{h.c.} \end{cases} \quad (6.78)$$

Note, however, that for the renormalizable term $\lambda H_u H_d \sigma^2$, without supersymmetry, one must fine-tune λ at order v_{ew}/f_a and M at order v_{ew}^2/f_a , which is the reason that the non-SUSY DFSZ model has a fine-tuning problem [58].

In any case, the axion is housed in the singlet σ , which has led to the so-called *invisible axion* physics. The effective interaction of the “invisible” axion can be written as, introducing the domain wall number N_{DW} ,

$$\begin{aligned} \mathcal{L}_\theta = & \frac{1}{2} f_S^2 \partial^\mu \theta \partial_\mu \theta - \frac{1}{4g_3^2} G_{\mu\nu}^a G^{a\mu\nu} + (\bar{q}_L i \not{D} q_L + \bar{q}_R i \not{D} q_R) \\ & + c_1 (\partial_\mu \theta) \bar{q} \gamma^\mu \gamma_5 q - (\bar{q}_L m q_R e^{ic_2 \theta} + \text{h.c.}) \\ & + c_3 \frac{\theta}{32\pi^2} G_{\mu\nu}^a \tilde{G}^{a\mu\nu} + c_{\theta\gamma\gamma} \frac{\theta}{32\pi^2} F_{\text{em},\mu\nu} \tilde{F}_{\text{em}}^{\mu\nu} + \mathcal{L}_{\text{leptons},\theta}, \end{aligned} \quad (6.79)$$

where $\tilde{F}_{\text{em}}^{\mu\nu} = \frac{1}{2} \epsilon^{\mu\nu\rho\sigma} F_{\text{em},\rho\sigma}$, $\theta = a/f_S$ with the axion decay constant f_S up to the domain wall number ($f_S = N_{\text{DW}} f_a$), g_3 is the QCD coupling, q is the fermion matrix composed of $\text{SU}(3)_c$ charge carrying fields, and m is the quark mass matrix. The domain wall number N_{DW} in the cosmos was presented in Section 5.3 and will be discussed shortly in several axion models. In the effective interaction of light fields, Eq. (6.79), only light fields are involved and the PQ symmetry is the shift symmetry of a . The c_1 term preserves the PQ symmetry. In the KSVZ model, the c_2 term is not present, but the anomaly term c_3 is present. In the DFSZ model, the anomaly term c_3 is not present, but the nonrenormalizable c_2 term provides the coupling of a to quarks and after one loop calculation with light quark loops, the needed anomaly term is generated. For axion physics, one usually writes the invisible axion coupling explicitly after calculating the loop integral. The useful terms are

$$\begin{aligned} \mathcal{L}_\theta = & \frac{1}{2} \partial^\mu a \partial_\mu a + \frac{g_3^2 c_3 a}{32\pi^2 f_a} G_{\mu\nu}^a \tilde{G}^{a\mu\nu} + c_{\theta\gamma\gamma} \frac{e^2 a}{32\pi^2} F_{\text{em},\mu\nu} \tilde{F}_{\text{em}}^{\mu\nu} \\ & + \frac{c_1}{N_{\text{DW}} f_a} (\partial_\mu a) \bar{q} \gamma^\mu \gamma_5 q - (\bar{q}_L m q_R e^{ic_2 a/N_{\text{DW}} f_a} + \text{h.c.}) + \mathcal{L}_{\text{leptons},\theta}. \end{aligned} \quad (6.80)$$

The “invisible” axion with a sufficiently large f_a can live very long. For it to be still alive, its mass is smaller than 24 eV. More detailed properties will be summarized in the following section.

Pontryagin index and domain wall number

Quantum chromodynamics¹⁰ is a gauge theory of gluons and quarks,

$$\mathcal{L}_{\text{QCD}} = -\frac{1}{2g_3^2} \text{Tr} G_{\mu\nu} G^{\mu\nu} + \bar{q}(i\not{D} - M)q, \quad (6.81)$$

where M is the diagonal matrix of quark masses, and $G_{\mu\nu}$ is the field strength matrix of gluon fields A_μ ,

$$\begin{aligned} G_{\mu\nu} &= \partial_\mu A_\nu - \partial_\nu A_\mu - i[A_\mu, A_\nu], \\ A_\mu &= \sum_a \left(\frac{\lambda^a}{2} \right) A_\mu^a, \\ \lambda^a &= \text{Gell-Mann matrices.} \end{aligned} \quad (6.82)$$

The pure gluon part of Eq. (6.81) has a classical solution [32], called instanton in the Euclidian spacetime. It is the self-dual (for instanton) or anti-self-dual (for anti-instanton) solution, satisfying, respectively,

$$\begin{aligned} G_{\mu\nu} &= \tilde{G}_{\mu\nu} \quad (\text{instanton}), \text{ or} \\ G_{\mu\nu} &= -\tilde{G}_{\mu\nu} \quad (\text{antiinstanton}). \end{aligned} \quad (6.83)$$

This solution has a topological number called Pontryagin index,

$$q = -\frac{1}{16\pi^2 g_3^2} \int d^4x \text{Tr} G_{\mu\nu} \tilde{G}^{\mu\nu} = -\frac{1}{32\pi^2 g_3^2} \int d^4x G_{\mu\nu}^a \tilde{G}^{a\mu\nu} > 0. \quad (6.84)$$

This was given before in Eq. (6.60) for general non-Abelian gauge theories. For an antiinstanton solution, q is negative. Because q is 1 for the simplest instanton, e^{iS} is identical to the previous one when one shifts $\bar{\theta}$ by 2π times integer where

$$S = -\frac{\bar{\theta}}{32\pi^2} \int d^4x G_{\mu\nu}^a \tilde{G}^{a\mu\nu}. \quad (6.85)$$

Hence, physics does not change by a shift of $\bar{\theta}$ by 2π , namely, the $\bar{\theta}$ periodicity is 2π . Comparing this with the axion coupling defined in Eq. (6.80), the gluon anomaly coupling defines f_a by the shift of $a \rightarrow a + 2\pi f_a$. But, Eq. (6.80) has another parameter N_{DW} which was defined as the VEV of scalar field, $f_S = N_{\text{DW}} f_a$, namely, the scalar field vacuum comes to itself only after the shift of $a \rightarrow a + N_{\text{DW}}(2\pi f_a)$. This is shown in Fig. 6.12 for $N_{\text{DW}} = 2$. Physical predictions are identical at the vacua with same color (red or blue in Fig. 6.12) in every aspect, including the ones related to nonanomalous couplings.

Cosmological aspects of domain walls was discussed in Section 5.3. It will be commented more in Section 6.6.

¹⁰Instead of gluodynamics, this word (including quark interactions) was suggested by P. Minkowski [59].

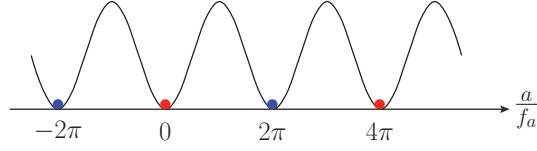


Fig. 6.12. The axion potential with minima at $\bar{\theta} = 2\pi n$, ($n = \text{integer}$), shown for $N_{\text{DW}} = 2$. At the same color vacua, physical predictions are identical in every aspect, including the ones related to nonanomalous couplings.

QCD axion as BCM

As soon as the bound on f_a of the invisible axion has been known [1], it was suggested that the invisible axion [2–5] is a candidate for filling the galaxies [47, 60]. It was the first example on BCM. Furthermore, the QCD axion, filling the halo, may behave like coherent collective motion discussed in Eqs. (6.40) and (6.42). If the invisible axion closes the Universe, in the beginning, f_a was estimated as 10^{12} GeV [1]. But, only 27% of the cosmic energy pie is CDM and hence f_a must be a bit smaller. Also, the anharmonic effect in the QCD axion in the estimation has been known to be significant [61, 62], and the current estimate on CDM axion density is given in Ref. [7], for $\Lambda_{\text{QCD}} = 380$ MeV,

$$\Omega_a = 0.025 \left(\frac{\theta_1^2 F(\theta_1)}{\gamma} \right) \left(\frac{0.68}{h} \right)^2 \left(\frac{f_a, \text{GeV}}{10^{11}} \right)^{1.184}, \quad (6.86)$$

where $g_{*,\text{present}} \simeq 3.91$ and γ is the entropy production ratio, and

$$\rho_c = 3.743 \times 10^{-11} \left(\frac{h}{0.68} \right)^2 \text{eV}^4. \quad (6.87)$$

For the numbers in the brackets of 1's, the QCD axion with $f_a = 10^{11}$ GeV constitutes 2.5% of the energy pie. If the QCD axion is one component among multi-components of CDM, for example with a ULA, then f_a of this order is expected [21].

Detection program of QCD axion

The local density of CDM is about 10^5 times larger than the critical density and close to 0.3 GeV cm^{-3} . The cavity detectors were proposed to detect these cosmic axions by haloscope. Also, the detection method of solar axions by helioscope was proposed [63]. Now, the calculation for the detection rate from axion-electrodynamics exists [64]. More on these will be presented in Chapter 9.

6.3.2. Discrete symmetries and axion mass

An axion starts from the Goldstone boson nature. Therefore, if the PQ symmetry at the Lagrangian level is exact, the axion is massless. This situation is illustrated

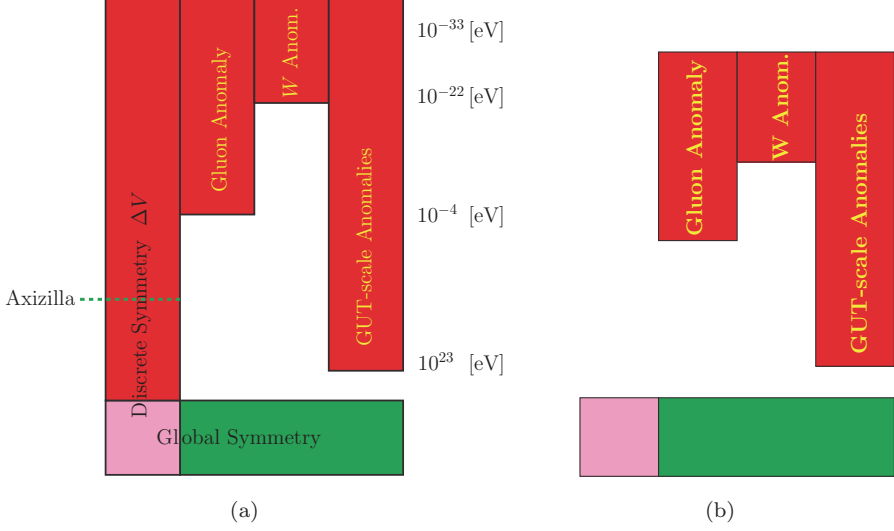


Fig. 6.13. The terms allowed by symmetries. (a) The terms in the far-left column are the terms in the potential V , which are allowed by discrete symmetries. The terms in the other columns arise from the anomalous terms. (b) This is the case when there are only anomalous terms.

in Fig. 6.13(a) by the effective terms where the green bar represents terms allowed by the PQ symmetry. If there is no term in the red, the axion is massless. Thus, the axion mass arises by the effects of breaking the PQ symmetry explicitly, by the terms in the reds in Fig. 6.13. For the vacuum to choose $\bar{\theta} = 0$ [57], the QCD anomaly term is present, not allowing any other term in the potential as depicted in Fig. 6.13(b).

There must be some terms defining the PQ symmetry, as shown in the lavender part of Fig. 6.13. For example, consider Eq. (6.68) for the PQWW axion. Without the c_{IJ} term, the PQ symmetry is defined. Then, it is broken by the c_{IJ} term in Eq. (6.68). For the DFSZ axion, with the reflection symmetry $\sigma \rightarrow -\sigma$ and Higgs doublet(s) $\rightarrow -\text{Higgs doublet(s)}$, we can consider

$$V_{\text{invisible}} = -\frac{1}{2}M^2\sigma^*\sigma + \frac{\lambda}{4}(\sigma^*\sigma)^2 + V(\text{e.w. Higgs}) + \Delta V + V_c(\sigma, \text{e.w. Higgs}), \quad (6.88)$$

where $V(\text{e.w. Higgs})$ is the Higgs potential for the electroweak symmetry breaking and $V_c(\sigma, \text{e.w. Higgs})$ is the coupling of the invisible axion singlet σ to Higgs doublet(s), and

$$\Delta V = \frac{\lambda_1}{4}\sigma^4 + \frac{\lambda_2}{4}\sigma^*\sigma^3 + \frac{1}{2}m_\epsilon^2\sigma^2 + \text{h.c.}$$

If any of λ_1, λ_2 and m_ϵ^2 are present, the PQ symmetry is broken. Also, the QCD anomaly term breaks the PQ symmetry. Thus, consider the terms breaking the PQ

symmetry, firstly for the case of two light quarks,

$$\mathcal{L} = -m_u(\bar{u}_R u_L + \bar{u}_L u_R) - m_d(\bar{d}_R d_L + \bar{d}_L d_R) - \frac{a}{f_a} \{G\tilde{G}\}, \quad (6.89)$$

where $\{G\tilde{G}\} \equiv \frac{1}{32\pi^2} G_{\mu\nu}^a \tilde{G}^{a\mu\nu}$. The dominant PQ symmetry violating term is written as the anomaly term. The quark mass terms give mass to π^0 also and hence a mixes with π^0 .

Assuming that $V_{\text{invisible}}$ respects the PQ symmetry, the QCD anomaly term is the only one explicitly breaking the PQ symmetry, which is depicted in Fig. 6.13(b). Let us calculate the axion mass in this case. The result is presented just before Section 6.3.3, after calculating the π^0 mass.

Mass of π mesons in chiral perturbation theory

When a is absent, by the partially conserved axial vector current (PCAC) hypothesis, the pseudo-Goldstone boson π^0 is written as the phase of $\bar{q}q$ condensate obtained from the nonvanishing divergence, $\partial_\mu J_5^{(3)\mu}$, where $J_5^{(3)\mu} = \frac{1}{2}\bar{u}\gamma^\mu\gamma_5 u - \frac{1}{2}\bar{d}\gamma^\mu\gamma_5 d$,

$$\langle \partial_\mu J_5^{(3)\mu} \rangle = m_u \langle \bar{u}i\gamma_5 u \rangle - m_d \langle \bar{d}i\gamma_5 d \rangle \propto \pi^0. \quad (6.90)$$

Consider three pions which form a triplet representation of the isospin group SU(2). Let us introduce the composite pseudoscalar Goldstone bosons as phases below the chiral symmetry breaking scale f , representing the chiral transformation as a shift of a pion π_i ,

$$\langle \bar{q}q \rangle \rightarrow \langle \bar{q}e^{i\gamma_5\pi_i/f}q \rangle + \frac{1}{2}\partial_\mu\pi^i\partial^\mu\pi^i, \quad (6.91)$$

where the last term converts the phases of the global symmetry as dynamical fields below the chiral symmetry breaking scale f . Then, the mass terms in Eq. (6.89) break the chiral symmetry, and render pions mass. The 2×2 quark mass matrix M generates the pion mass-squared matrix $\mathcal{M}$,

$$\Delta\mathcal{H}^{(\text{mass})} = m_u\bar{u}u + m_d\bar{d}d = \bar{q} \begin{pmatrix} m_u & 0 \\ 0 & m_d \end{pmatrix} q \rightarrow \frac{1}{2}\pi^\dagger \mathcal{M} \pi. \quad (6.92)$$

Using (6.91), we obtain

$$\frac{1}{2}\pi^\dagger \mathcal{M} \pi = \left\langle \bar{q}e^{i\gamma_5 T_i \pi_i/f} \begin{pmatrix} m_u & 0 \\ 0 & m_d \end{pmatrix} e^{i\gamma_5 T_j \pi_j/f} q \right\rangle, \quad \text{with } T_i = \frac{1}{2}\sigma_i. \quad (6.93)$$

Choose the SU(2) shift direction defined by directional cosines $\cos^2\theta_1 + \cos^2\theta_2 + \cos^2\theta_3 = 1$ such that $\vec{\sigma}^2 = \mathbf{1}$, where

$$\tilde{\pi} = \cos\theta_1\pi_1 + \cos\theta_2\pi_2 + \cos\theta_3\pi_3, \quad (6.94)$$

$$\tilde{\sigma} = \cos\theta_1\sigma_1 + \cos\theta_2\sigma_2 + \cos\theta_3\sigma_3. \quad (6.95)$$

Thus, Eq. (6.93) can be

$$\begin{aligned}
\frac{1}{2}\pi^\dagger \mathcal{M}\pi &= \left\langle \bar{q} \left(\mathbf{1} \cos \frac{\tilde{\pi}}{2f} + i\gamma_5 \tilde{\sigma} \sin \frac{\tilde{\pi}}{2f} \right) (\bar{m}\mathbf{1} - \Delta\sigma_3) \right. \\
&\quad \times \left. \left(\mathbf{1} \cos \frac{\tilde{\pi}}{2f} + i\gamma_5 \tilde{\sigma} \sin \frac{\tilde{\pi}}{2f} \right) q \right\rangle \\
&= \bar{m} \langle \bar{q}_i(\sigma_\alpha)_{ik} \cos \theta_\alpha i\gamma_5 q_k \rangle \sin \frac{\tilde{\pi}}{f} - \bar{m} \langle \bar{q}_i q_i \rangle \sin^2 \frac{\tilde{\pi}}{2f} \\
&\quad - \bar{m} i\epsilon_{\alpha\beta\gamma} \cos \theta_\alpha \cos \theta_\beta \langle \bar{q}_i(\sigma_\gamma)_{ik} q_k \rangle \sin^2 \frac{\tilde{\pi}}{2f},
\end{aligned} \tag{6.96}$$

where

$$\begin{aligned}
\bar{m} &= \frac{m_u + m_d}{2}, \quad \Delta = \frac{m_d - m_u}{2}, \\
m_1 &= m_u = \bar{m} - \Delta, \quad m_2 = m_d = \bar{m} + \Delta.
\end{aligned} \tag{6.97}$$

The PCAC direction is related to the pion Goldstone boson direction by the extremum condition on (6.96),

$$\begin{aligned}
&\langle \bar{q}_i(\sigma_\alpha)_{ik} i\gamma_5 q_k \rangle \cos \theta_\alpha \cos \frac{\tilde{\pi}}{2f} \\
&= (2\langle \bar{q}_i q_i \rangle + i\epsilon_{\alpha\beta\gamma} \cos \theta_\alpha \cos \theta_\beta \langle \bar{q}_i(\sigma_\gamma)_{ik} q_k \rangle) \sin \frac{\tilde{\pi}}{2f}.
\end{aligned}$$

Strong interaction dynamics is assumed not to break the isospin symmetry, and hence we obtain

$$\langle \bar{q}_i(\sigma_\alpha)_{ik} i\gamma_5 q_k \rangle \cos \theta_\alpha = 2\langle \bar{q}_i q_i \rangle \tan \frac{\tilde{\pi}}{2f}. \tag{6.98}$$

Integrating out the quark fields in Eq. (6.96),

$$V = \frac{1}{2}\pi^\dagger \mathcal{M}\pi = \bar{m}\Lambda_{\text{QCD}}^3 \sin^2 \frac{\tilde{\pi}}{2f}, \tag{6.99}$$

where $\Lambda_{\text{QCD}}^3 = \langle \bar{q}_i q_i \rangle$. The pion mass matrix calculated near $\tilde{\pi} = 0$ is

$$\mathcal{M}_{ij} = \frac{\partial^2 V}{\partial \pi_i \partial \pi_j} \Big|_{\tilde{\pi}=0} = \frac{\bar{m}\Lambda_{\text{QCD}}^3}{f^2} \cos^2 \frac{\tilde{\pi}}{2f} (\cos \theta_i \cos \theta_j) \Big|_{\tilde{\pi}=0}, \tag{6.100}$$

so that we obtain the identical mass for $\pi^\pm$ and π^0 . In this way, the pion mass in the chiral perturbation theory is obtained:

$$m_\pi^2 = \frac{(m_u + m_d) \Lambda_{\text{QCD}}^3}{2f_\pi^2}, \tag{6.101}$$

where we set $f = f_\pi$. The mass difference of $\pi^\pm$ and π^0 is due to the isospin breaking by Δ and electromagnetism.

So far, we worked only in the SU(2) isospin space where the sigma-matrix algebra is rather simple. In low energy phenomenology, however, we consider SU(3) flavor space where we must consider eight λ matrices instead of three σ matrices. This extension introduces some complication. But the method is the same. Let us note how the assumptions we invoked above can be extended:

- (1) If the flavor space is extended, the additional current quark masses are no longer as small as m_u and m_d . Then, the universal parameters we introduced for the condensation scale Λ_{QCD} and decay constant f might be no longer universal, and we can consider the following types for the corresponding matrices:

$$\left(\begin{array}{cc|c} x & x & y \\ x & x & y \\ \hline - & - & - \\ y & y & z \end{array} \right),$$

where the isospin invariance is required to be satisfied.

- (2) One may assume that $\langle \bar{q}q \rangle = \Lambda_{\text{QCD}}^3$ and different decay constants $f_{\pi_i \pi_j} = \{f, f_{\pi_i s}, f_{ss} = f_s\}$. Under this assumption, the upper bound of $m_{\eta'} \leq \sqrt{3}m_\pi$ was obtained [31].
- (3) One may assume that decay constants are universally f and different values for quark condensation values, $\langle \bar{q}q \rangle = \{\Lambda_{\text{QCD}}^3, \Lambda_{\text{QCD},s}^3, \Lambda_{s,s}^3\}$. Because the mass of the strange quark s is ~ 100 MeV and $\Lambda_{\text{QCD}} \simeq 380$ MeV, it makes sense to assume different quark condensation scales.
- (4) One may assume that both condensation values and decay constants are not universal.

If we take items (3) and (4), the η' mass bound may not be necessarily $m_{\eta'} \leq \sqrt{3}m_\pi$. We point out that item (3) is most promising in the sense that the shift of angle $a_i/f_i \rightarrow a_i/f_i + 2\pi$ is a discrete symmetry and all pseudo-Goldstone bosons are treated in the same way.

Solution of the U(1) problem

Without the anomaly term, we encounter the severe phenomenological problem, the so-called U(1) problem [31]. Assuming item (3), we use the same decay constant f with $\bar{\theta} = \eta'/f$, and now we include the anomaly term in the Hamiltonian

$$\mathcal{H} = \frac{1}{2}\pi^\dagger \mathcal{M} \pi + \frac{\eta'}{f} \{G\tilde{G}\}, \quad (6.102)$$

where

$$\frac{1}{2}\pi^\dagger \mathcal{M}\pi = \left\langle \bar{q} e^{i\gamma_5 F_a \pi_a / f} \begin{pmatrix} m_u & 0 & 0 \\ 0 & m_d & 0 \\ 0 & 0 & m_s \end{pmatrix} e^{i\gamma_5 F_b \pi_b / f} q \right\rangle, \\ \text{with } F_a = \frac{1}{2}\lambda_a. \quad (6.103)$$

We can integrate out gluons, which is equivalent to applying a chiral U(1) transformation $q \rightarrow e^{i\gamma_5 \bar{\theta}} q$. It is equivalent to considering the following mass term:

$$\frac{1}{2}\pi^\dagger \mathcal{M}\pi = \left\langle \bar{q} e^{i\gamma_5 (F_a \pi_a / f - \eta' / 2f)} \begin{pmatrix} m_u & 0 & 0 \\ 0 & m_d & 0 \\ 0 & 0 & m_s \end{pmatrix} e^{i\gamma_5 (F_b \pi_b / f - \eta' / 2f)} q \right\rangle \\ \equiv \langle \bar{q} \mathbf{e} M \mathbf{e} q \rangle, \quad (6.104)$$

where

$$\mathbf{e} = e^{i\gamma_5 (F_b \pi_b / f - \eta' / 2f)}. \quad (6.105)$$

Note that the phase contains the factor

$$(\lambda_a \pi_a - \eta' \mathbf{1}) = \begin{pmatrix} \pi_3 + \frac{1}{\sqrt{3}}\eta - \eta', & \pi_1 - i\pi_2, & \pi_4 - i\pi_5 \\ \pi_1 + i\pi_2, & -\pi_3 + \frac{1}{\sqrt{3}}\eta - \eta', & \pi_6 - i\pi_7 \\ \pi_4 + i\pi_5, & \pi_6 + i\pi_7, & -\frac{2}{\sqrt{3}}\eta - \eta' \end{pmatrix}. \quad (6.106)$$

Near $\pi_i = 0$ and $\eta' = 0$, we can express the derivatives as

$$\frac{\partial}{\partial \varphi_x} \langle \bar{q} \mathbf{e} M \mathbf{e} q \rangle = \frac{i}{2f} \langle \bar{q} \mathbf{e} \gamma_5 (\lambda_a \delta_{\pi_a \varphi_x} - \delta_{\eta' \varphi_x}) M \mathbf{e} q \rangle \\ + \frac{i}{2f} \langle \bar{q} \mathbf{e} M (\lambda_a \delta_{\pi_a \varphi_x} - \delta_{\eta' \varphi_x}) \gamma_5 \mathbf{e} q \rangle, \quad (6.107)$$

where fields are only in the exponent. Therefore, the mass matrix is

$$\frac{\partial^2}{\partial \varphi_y \partial \varphi_x} \langle \bar{q} \mathbf{e} M \mathbf{e} q \rangle \Big|_0 = -\frac{1}{4f^2} \langle \bar{q} (\lambda_a \delta_{\pi_a \varphi_y} - \delta_{\eta' \varphi_y}) (\lambda_a \delta_{\pi_a \varphi_x} - \delta_{\eta' \varphi_x}) M q \rangle \\ -\frac{1}{4f^2} \langle \bar{q} (\lambda_a \delta_{\pi_a \varphi_x} - \delta_{\eta' \varphi_x}) M (\lambda_a \delta_{\pi_a \varphi_y} - \delta_{\eta' \varphi_y}) q \rangle \\ -\frac{1}{4f^2} \langle \bar{q} (\lambda_a \delta_{\pi_a \varphi_y} - \delta_{\eta' \varphi_y}) M (\lambda_a \delta_{\pi_a \varphi_x} - \delta_{\eta' \varphi_x}) q \rangle \\ -\frac{1}{4f^2} \langle \bar{q} M (\lambda_a \delta_{\pi_a \varphi_x} - \delta_{\eta' \varphi_x}) (\lambda_a \delta_{\pi_a \varphi_y} - \delta_{\eta' \varphi_y}) q \rangle. \quad (6.108)$$

For example, for φ_1 and φ_1 , we have

$$\begin{aligned} \left. \frac{\partial^2}{\partial \varphi_1 \partial \varphi_1} \langle \bar{q} \mathbf{e} M \mathbf{e} q \rangle \right|_0 &= -\frac{1}{4f^2} \langle \bar{q} \lambda_1^2 (\bar{m} - \Delta \lambda_3) q \rangle - \frac{1}{4f^2} \langle \bar{q} \lambda_1 M \lambda_1 q \rangle \\ &\quad - \frac{1}{4f^2} \langle \bar{q} \lambda_1 M \lambda_1 q \rangle - \frac{1}{4f^2} \langle \bar{q} (\bar{m} - \Delta \lambda_3) \lambda_1^2 q \rangle \\ &= -\frac{4\bar{m}}{4f^2} \langle \bar{q} q \rangle = \frac{(m_u + m_d) \Lambda_{\text{QCD}}^3}{2f^2}, \end{aligned} \quad (6.109)$$

while for φ_1 and φ_2 , we have 0. Equation (6.109) gives the $\pi^\pm$ mass given in Eq. (6.101). Equipped with this, we differentiate with respect to η' to obtain

$$\begin{aligned} \left. \frac{\partial^2}{\partial \eta' \partial \eta'} \langle \bar{q} \mathbf{e} M \mathbf{e} q \rangle \right|_0 &= -\frac{4}{4f^2} \left\langle \bar{q} \begin{pmatrix} \bar{m} - \Delta \sigma_3 & 0 \\ 0 & m_s \end{pmatrix} q \right\rangle \\ &= -\frac{\bar{m}}{f^2} \langle \bar{u}u + \bar{d}d \rangle - \frac{m_s}{f^2} \langle \bar{s}s \rangle = m_\pi^2 + \frac{m_s \Lambda_s^3}{2f^2}. \end{aligned} \quad (6.110)$$

Taking the view of item 3, we take $f \simeq 93$ MeV, $m_s \simeq 100$ MeV. Then, $m_{\eta'} \simeq 958$ MeV is fitted with $\Lambda_s \simeq 427$ MeV. In Eq. (6.110), the first term had led to the U(1) problem [31] and the second term, which arises from the anomaly, is the solution of the U(1) problem as suggested by 't Hooft [34].

VEV of π^0 in the $\bar{\theta}$ -vacuum

The term $\bar{\theta}\{G\tilde{G}\}$ looks like the η' term in Eq. (6.102). Then, by redefining $\eta' + \bar{\theta} \rightarrow \eta'$, Eq. (6.106) does not contain $\bar{\theta}$, and it seems that there is no strong CP problem. If it were true, there would be no strong CP problem. But, one cannot remove the strong CP problem by redefining $\eta' + \bar{\theta}f \rightarrow \eta'$. The reason is the following. Below the confinement scale, we must consider the baryon octet, N , also. Its coupling to η' is

$$f_{NN\eta'} \bar{N} i \gamma_5 N \eta'. \quad (6.111)$$

Assuming $\bar{\theta}$ is small, let us work first in the meson vacuum where $\langle \pi^0 \rangle = 0$ and $\langle \eta' \rangle = 0$ and all masses are real and positive. If we redefine η' to remove $\bar{\theta}$, the $f_{NN\eta'}$ coupling introduces $-f_{NN\eta'} f \bar{\theta} \bar{N} i \gamma_5 N$ which is not consistent with the real and positive baryon masses. Therefore, $\bar{\theta}$ cannot be removed by redefining $\eta' + \bar{\theta} \rightarrow \eta'$. Again, we conclude that the strong CP problem is a real physical problem.

Let us consider $\mathbf{e}$ with the unremovable $\bar{\theta}$,

$$\mathbf{e} = e^{i\gamma_5 \frac{1}{2}(\lambda_b \pi_b / f - \eta' / f - \bar{\theta})}. \quad (6.112)$$

At the meson vacuum, we have $\mathbf{e} \simeq e^{-i\gamma_5 \frac{1}{2}\bar{\theta}}$. The term $\mathcal{H}$ that we considered in (6.102) is the chiral symmetry breaking term to generate meson masses such as

$\frac{1}{2}m_{\pi_i}^2\pi_i^2 + \dots$. Thus, the VEV of π^0 is determined, for a small $\bar{\theta}$, by

$$\begin{aligned} m_{\pi_i}^2\pi_i &\simeq -(\text{Eq. (6.107)}) \text{ for } \pi_i = \pi^0 \text{ with zero meson VEVs} \\ &= \frac{\bar{\theta}\Delta}{f}\langle\bar{q}q\rangle = \frac{\bar{\theta}\Delta\Lambda_{\text{QCD}}^3}{f}, \end{aligned} \quad (6.113)$$

giving the VEV of π^0 in the $\bar{\theta}$ -vacuum,

$$\langle\pi^0\rangle = \frac{\Delta\Lambda_{\text{QCD}}^3}{f m_{\pi^0}^2} \bar{\theta}. \quad (6.114)$$

Since π^0 has the CP eigenvalue -1 , this breaks the CP symmetry and is the dominant source for the NEDM in the $\bar{\theta}$ -vacuum [37].

Axion mass

Thus, the “invisible” axion solution seems to be the remaining solution. It is based on the potential,

$$V_{\text{axion}} \simeq f_{\pi^0}^2 m_{\pi^0}^2 \frac{Z}{(1+Z)^2} \left(1 - \cos \frac{a}{f_a}\right), \quad (6.115)$$

where $Z = m_u/m_d$. This potential is derived by introducing the axion coupling $(a/f_a)\{G\tilde{G}\}$ as we have practised above. Along the way, one must make a orthogonal to π^0 and η' . It gives the axion mass [47, 65, 66]

$$m_a = \frac{\sqrt{Z}}{1+Z} \frac{f_{\pi^0}^2 m_{\pi^0}^2}{f_a^2} \simeq 0.61 [\text{eV}] \times \frac{10^7 \text{ GeV}}{f_a}. \quad (6.116)$$

6.3.3. Classification of QCD axions

The invisible axion a , a pseudoscalar, resides in the phase of a nonzero PQ-charged (complex and neutral) SM singlet field(s) σ [2]. In a broader sense, a is defined to have a continuous shift symmetry,

$$a \rightarrow a + \text{constant}. \quad (6.117)$$

The antisymmetric tensor field B_{MN} in string theory is also called axions [67–70]. In the sense of (6.117), all light pseudoscalars can be called axions. Indeed, many GUT scale pseudoscalars are called axions, in particular those used in N -flation models [26]. Also, if it is very light, it is called axion-like particles (ALPs). But the original definition of axion was to have an anomaly [46], i.e., a nonvanishing $\text{U}(1)_{\text{PQ}}\text{-SU}(N)\text{-SU}(N)$ anomaly where $\text{SU}(N)$ is a non-Abelian gauge group. Among non-Abelian groups in the SM, only the color force is important because we live in the region where the color coupling is large. The $\text{SU}(2)_W$ effect to the axion is extremely small, $\sim e^{-8\pi^2/g_s^2}$, which is sketched roughly as the W -anomaly line 10^{-22} eV in

Fig. 6.13(a). In this book, we follow this wide use of “axion”, which is basically “pseudoscalar”.

Now, we call the “invisible” axion having the color anomaly the *QCD axion*.

By PQ charged quarks

Depending on how the QCD anomaly is introduced, it is called either the KSVZ axion or the DFSZ axion. If the anomaly is introduced by a heavy quark, it is called the KSVZ axion [2, 3], and if the anomaly is introduced by the SM quarks, it is called the DFSZ axion [4, 5]. This distinction is only for an eyeball number for the couplings. One expects that the “invisible” axion include the effects of all PQ charged quarks, which is a general case from string compactification. In any attempt to obtain the “invisible” axion component from superstring, contributions from both heavy quarks and SM quarks are present [71, 73].

By the misalignment angle

The “invisible” axion is also classified by the size of the misalignment angle θ_1 , a natural one with $\theta_1 = O(1)$ and a fine-tuned one with $\theta_1 \ll 1$. [Note, however, the bottleneck period discussed in Section 6.1 and the corresponding θ_2 .] The natural one renders a possibility of discovery, but the fine-tuned one is not so easy to be discovered:

$$\theta_1 = O(1): 10^9 \text{ GeV} \lesssim f_a \lesssim 10^{11} \text{ GeV}, \quad (6.118)$$

$$\theta_1 \ll 1: f_a \gtrsim 10^{12} \text{ GeV}. \quad (6.119)$$

The fine-tuned ones employ the anthropic scenario for its realization in cosmology [74, 75].

6.3.4. Axion–photon–photon coupling

The “invisible” axion may be detected by the cavity resonators with strong magnetic field. The coupling $c_{a\gamma\gamma}$ is defined by

$$-c_{a\gamma\gamma} \frac{\alpha_{\text{em}}}{2\pi} \mathbf{E}_{\text{em}} \cdot \mathbf{B}_{\text{em}} \frac{a}{f_a}, \quad (6.120)$$

where $c_{a\gamma\gamma}$ is composed of two parts:

$$c_{a\gamma\gamma} \simeq c_{a\gamma\gamma}^0 - 2, \quad (6.121)$$

where $c_{a\gamma\gamma}^0$ is the one determined by the model, and -2 is the approximate shift due to the QCD chiral symmetry breaking for $Z = m_u/m_d = 0.5$. Depending on the ratio m_u/m_d , -1.91 [47] and -1.98 [37] were used before. The details on the detection methods will be discussed in Chapter 9, and here we present the theoretical bases of calculating $c_{a\gamma\gamma}$.

The chiral symmetry breaking effect is calculated before [47], and here we use the low energy Lagrangian of Eq. (6.80), and integrating out the gluon fields, we obtain

$$\begin{aligned} \mathcal{L}_\theta = & \frac{1}{2} \partial^\mu a \partial_\mu a + c_{\theta\gamma\gamma} \frac{e^2 a}{32\pi^2 f_a} F_{\mu\nu}^{\text{em}} \tilde{F}_{\text{em}}^{\mu\nu} + \frac{c_1}{N_{\text{DW}} f_a} (\partial_\mu a) \bar{q} \gamma^\mu \gamma_5 q \\ & - (\bar{q}_L m q_R e^{i(c_2+c_3)a/N_{\text{DW}} f_a} + \text{h.c.}) + \mathcal{L}_{\text{leptons}, \theta}. \end{aligned} \quad (6.122)$$

We define the axion a and f_a by all PQ charged quarks such that $c_2 + c_3 = 1$. In Eq. (6.122), the invariant axionic domain wall number is N_{DW} [37]. Thus, we can consider the following hadronic interaction with $\theta_a \equiv a/f_a$:

$$\mathcal{L}[a, u, d] = -\frac{1}{4e^2} F_{\mu\nu}^{\text{em}} F_{\text{em}}^{\mu\nu} - (\bar{q}_L m q_R e^{i\theta_a/N_{\text{DW}}} + \text{h.c.}), \quad (6.123)$$

where m is the 2×2 mass matrix. Now, to make the quark mass matrix real and positive, let us transform away the phase θ_a from the quarks, which then goes into the coupling $(a/f_a)\{F_{\mu\nu}^{\text{em}} \tilde{F}_{\text{em}}^{\mu\nu}\}$. The PCAC currents related to π mesons is J_5^μ whose divergence is the interpolating pion fields, given in Eq. (6.98). Thus, the axion must be orthogonal to $\pi^0 \propto m_u \bar{u} i \gamma_5 u - m_d \bar{d} i \gamma_5 d$, neglecting the heavier quarks s, c , etc., implying

$$\theta_a \propto m_d \bar{u} i \gamma_5 u + m_u \bar{d} i \gamma_5 d \propto \frac{\bar{u} i \gamma_5 u + Z \bar{d} i \gamma_5 d}{1 + Z}. \quad (6.124)$$

Thus, the axion coupling to u, d quarks are $\frac{1}{1+Z}, \frac{Z}{1+Z}$, respectively. The sign is opposite to those calculating $\tilde{c}_{a\gamma\gamma}$ because we transform away the phase,

$$-2 \cdot 3 \left[\frac{1}{1+Z} \left(\frac{2}{3} \right)^2 + \frac{Z}{1+Z} \left(-\frac{1}{3} \right)^2 \right] = -2 \quad \text{for } Z = 0.5. \quad (6.125)$$

In the KSVZ axion model, $c_{a\gamma\gamma}^0$ is determined by the PQ charge carrying heavy fermions. If there is only one neutral quark for this, then $c_{a\gamma\gamma}^0$ would be zero. If there is only one PQ charge carrying heavy quark with the electromagnetic charge Q_{em} , then $c_{a\gamma\gamma}^0 \propto Q_{\text{em}}^2$. The proportionality factor must take into account the L- and R-handed and also color degrees of freedom, where the PQ charge of the singlet σ is defined to be 1. But, in realistic models from a fundamental theory, it is more likely that there exist many PQ charge carrying quarks and leptons. Thus, the couplings given for one heavy quark in Table 6.1 are presented just as for an illustration.

In the DFSZ model, we consider only light quarks and leptons of the SM for the fermions. The PQ charges of H_u and H_d determine the PQ charges of u and d quarks. For the PQ charge of electron e , we have two possibilities: H_d gives mass to

Table 6.1. The KSVZ models with $m_u = 0.5 m_d$. (m, m) in the last row means m quarks of $Q_{\text{em}} = \frac{2}{3} e$ and m quarks of $Q_{\text{em}} = -\frac{1}{3} e$.

KSVZ: Q_{em}	$c_{a\gamma\gamma}$
0	-2
$\pm \frac{1}{3}$	$-\frac{4}{3}$
$\pm \frac{2}{3}$	$+\frac{2}{3}$
± 1	+4
(m, m)	$-\frac{1}{3}$

Table 6.2. The DFSZ models with $m_u = 0.5 m_d$. The non-SUSY DFSZ models have a fine-tuning problem. A related cosmological problem even within SUSY framework was pointed out in [58].

DFSZ: $(q^c - e_L)$ pair	Higgs	$c_{a\gamma\gamma}$
non-SUSY (d^c, e)	H_d	$+\frac{2}{3}$
non-SUSY (u^c, e)	H_u^*	$-\frac{4}{3}$
GUTs		$+\frac{2}{3}$
SUSY		$+\frac{2}{3}$

e and the PQ charge of e is the same as that of d , or H_u gives mass to e and then the PQ charge of e is the opposite to that of u :

$$\begin{aligned}
 c_{a\gamma\gamma}^0 &= +\frac{2v_d^2}{v_{EW}^2} \left(\frac{2}{3}\right)^2 \cdot 3 + \frac{2v_u^2}{v_{EW}^2} \left[\left(-\frac{1}{3}\right)^2 \cdot 3 + (-1)^2\right] \\
 &= +\frac{8}{3}, \quad \text{electron mass by } H_d,
 \end{aligned} \tag{6.126}$$

$$\begin{aligned}
 c_{a\gamma\gamma}^0 &= +\frac{2v_d^2}{v_{EW}^2} \left[\left(\frac{2}{3}\right)^2 \cdot 3 - (-1)^2\right] + \frac{2v_u^2}{v_{EW}^2} \left(-\frac{1}{3}\right)^2 \cdot 3 \\
 &= +\frac{2}{3}, \quad \text{electron mass by } H_u^\dagger.
 \end{aligned} \tag{6.127}$$

The PQ charges of $H_{u,d}$ are chosen to be negative, i.e., negative of that of σ . So, we choose the PQ charges of light quarks to be positive in (6.126) and (6.127). For the PQWW axion, the coupling is the same as those of (6.126) and (6.127) except the overall signs. The $c_{a\gamma\gamma}$ values for the DFSZ models are presented in Table 6.2.

6.3.5. $c_{a\gamma\gamma}^0$ from string

When the PQ symmetry, $U(1)_{\text{PQ}}$, is spontaneously broken at the scale f_a , it introduces one loop $U(1)_{\text{PQ}}\text{--}SU(3)_c\text{--}SU(3)_c$ anomaly which translates to the axion's coupling to the gluon anomaly

$$\frac{1}{2\pi} \sum_{\alpha=1}^8 \mathbf{E}_{\text{gluon}}^\alpha \cdot \mathbf{B}_{\text{gluon}}^\alpha \frac{a}{f_a}. \quad (6.128)$$

The axion–photon–photon coupling of Eq. (6.120) is normalized with the above definition on the QCD axion, which is consistent with Eq. (6.62).

We use the index ℓ normalization such that the fundamental representation of $SU(N)$ has $\ell = \frac{1}{2}$. Then, the indices of some $SU(N)$ representations are

$$SU(N): \quad 2\ell(\mathbf{N}) = 1, \quad 2\ell([2]) = N - 2, \quad 2\ell([3]) = \frac{(N-2)(N-3)}{2}, \quad (6.129)$$

$$2\ell(\text{Adj.}) = 2N, \quad 2\ell(\{2\}) = N + 2, \quad (6.130)$$

$$2\ell(\{3\}) = \frac{(N+2)(N+3)}{2}, \quad (6.131)$$

$$U(1)_{\text{em}}: \quad 2\ell(Q_{\text{em}}) = 2Q_{\text{em}}^2, \quad (6.132)$$

where $[2]$ means the dimension $\left(\frac{N(N-1)}{2!}\right)$ with two antisymmetric indices, $\{2\}$ means the dimension $\left(\frac{N(N+1)}{2!}\right)$ with two symmetric indices, $[3]$ means the dimension $\left(\frac{N(N-1)(N-2)}{3!}\right)$ with three antisymmetric indices, etc.

In string models, some discrete symmetries are allowed, but global symmetries are not. In the far left column of Fig. 6.13(a), we depict this situation as the allowed terms by some discrete symmetry from string compactification. If we consider a few leading terms among them as shown with the lavender part, there may appear some global symmetries as symbolized with the green bar in the figure. Thus, the terms corresponding to the lavender part define a PQ symmetry, for example. In Ref. [76], the first seven terms in the potential in the model of Ref. [77] were considered, which belong to the lavender part and allowed a PQ symmetry. For this model, $c_{a\gamma\gamma}$ was calculated, which is presented in Table 6.3.

The trace of Q_{em}^2 for an anomaly-free irreducible set, including the fundamental representation of GUT representations, defines $\sin^2 \theta_W^0$ of that GUT [73]. From this trace, we can find out the axion–photon–photon coupling also. Note that the

Table 6.3. String model. Comments are for $U(1)_{\text{PQ}}$. In the last row, $c_{a\gamma\gamma} = (1 - 2\sin^2 \theta_W)/\sin^2 \theta_W$ with $m_u = 0.5m_d$.

String:	$c_{a\gamma\gamma}$	Comments
Ref. [76]	$-\frac{1}{3}$	Approximate
Refs. [73, 78]	$+\frac{2}{3}$	Anom. $U(1)$

unification assumption is crucial here. Let Q_{PQ} be the PQ charge operator. Let us compare $\text{Tr } Q_{\text{PQ}} Q_{\text{em}}^2$ to $\text{Tr } Q_{\text{PQ}}(\text{color couplings})$. The ratio gives the coupling $c_{a\gamma\gamma}^0$. The model-independent (MI) axion from superstring [68, 69] is shown as the white square in the upper left corner in Fig. 9.11.

6.3.6. With anomalous $U(1)$ and 't Hooft mechanism

For the anomalous $U(1)$ in string theory, all the charges of massless fermions in compactification carries the same eigenvalue of Q_{PQ} . Therefore, it is equivalent to calculating

$$c_{a\gamma\gamma}^0 = \frac{2 \text{Tr } Q_{\text{PQ}} Q_{\text{em}}^2}{\sum_{\text{quarks}} Q_{\text{PQ}} \ell(\text{quarks})} = \frac{N}{D}. \quad (6.133)$$

Since $Q_{\text{em}} = T_3 + Y$, we have

$$\text{Tr } Q_{\text{em}}^2 = \text{Tr } T_3^2 + \text{Tr } Y^2 = \text{Tr } T_3^2 + 2\eta^2 \text{Tr } \tilde{Y}^2, \quad (6.134)$$

where $\text{Tr } T_3^2 = \frac{1}{2}$ for one doublet and $Y = \eta \tilde{Y}$ in terms of properly normalized $\tilde{Y}$ in GUTs. Now, N and D of Eq. (6.133) are

$$N = \sum_{\text{weak nonsinglets}} Q_{\text{PQ}} \ell + \sum_{\text{weak singlets}} 2\eta^2 \text{Tr } Q_{\text{PQ}} \tilde{Y}^2, \quad (6.135)$$

$$D = \sum_{\text{color nonsinglets}} Q_{\text{PQ}} \ell(\text{quarks}), \quad (6.136)$$

where factor 2 for indices of $U(1)$ in (6.132) is taken into account and we used Eq. (6.134). For the anomalous $U(1)$ from the Green-Schwarz (GS) term [67] in string compactification, $\text{Tr } Q_{\text{PQ}} F_G^2$, where F_G is the fundamental representation generator of a non-Abelian group, is the same for any non-Abelian group and a properly normalized $U(1)$ charge operator $\tilde{Y}$,

$$\sum_{\text{weak nonsinglets}} Q_{\text{PQ}} \ell = \sum_{\text{color nonsinglets}} Q_{\text{PQ}} \ell(\text{quarks}) = \text{Tr } \tilde{Y}^2. \quad (6.137)$$

Thus, we obtain

$$c_{a\gamma\gamma}^0 = 1 + 2\eta^2. \quad (6.138)$$

Therefore, if all PQ charges of the fermions are the same as in the anomalous $U(1)$ case, we have the simple form (6.138). If GUTs give no funnily charged quarks, then we obtain $c_{a\gamma\gamma}^0 = \frac{8}{3}$. If funnily charged fermions are present, $c_{a\gamma\gamma}^0$ is no longer $\frac{8}{3}$.

In models where the anomalous $U(1)$ becomes $U(1)_{\text{PQ}}$ at low energy, Eq. (6.138) applies. For example, Ref. [71] gives $\text{Tr } Q_{\text{em}}^2 = 60$. (Note the number was 2160 which was multiplied the result by 6^2 .) In the compactification example without funnily charged fermions, we can check that $c_{a\gamma\gamma}^0 = \frac{8}{3}$ [73]. In the model presented in

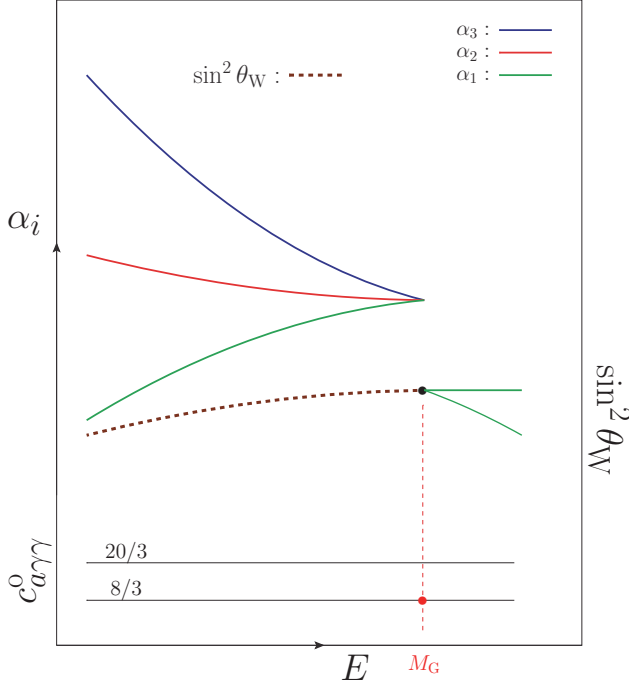


Fig. 6.14. A schematic view on the gauge couplings, $\sin^2 \theta_W$, and $c_{a\gamma\gamma}^0$. The evolution of $\sin^2 \theta_W$ is shown in the middle part. $c_{a\gamma\gamma}^0$ is determined by quantum numbers and does not evolve as shown in the lower part for $\frac{20}{3}$ and $\frac{8}{3}$.

Ref. [73], we know all spectra, and we calculate $c_{a\gamma\gamma}^0$ directly from (6.133), instead of (6.138),

$$c_{a\gamma\gamma}^0 = \frac{\sum_{\text{charged fermions}} Q_{PQ} Q_{\text{em}}^2}{\sum_{\text{quarks}} Q_{PQ} \ell(\text{quarks})} = \frac{-9312}{-3492} = \frac{8}{3}. \quad (6.139)$$

Calculation of $c_{a\gamma\gamma}^0$ depends on the quantum numbers which do not evolve. So, it is constant once the Q_{PQ} and electromagnetic charges are known for all the fermions in the theory. On the other hand, $\sin^2 \theta_W$ evolves as shown in Fig. 6.14. Suppose that below M_{GUT} there is no funnily charged fermions as in the spectrum from $\text{SO}(10)$ GUT. Then, the evolution of coupling from the observed α 's at the electroweak scale meets at M_{GUT} . If there are more charged fermions above M_{GUT} , two cases can be considered. If these vector-like particles form $\text{SO}(10)$ representations, then $\sin^2 \theta_W$ remains as $\frac{3}{8}$ above M_{GUT} as shown with the green line. If the charged fermions above the GUT do not form $\text{SO}(10)$ representations, $\sin^2 \theta_W$ evolves to a smaller value above M_{GUT} as shown with the green curve.

Table 6.3 provides a summary of $c_{a\gamma\gamma}$ in string compactifications. The unification condition, giving $c_{a\gamma\gamma} = \frac{8}{3}$, is illustrated as the thick black line in Fig. 6.15. However, the unification condition is neglecting the PQ charged GUT singlets above

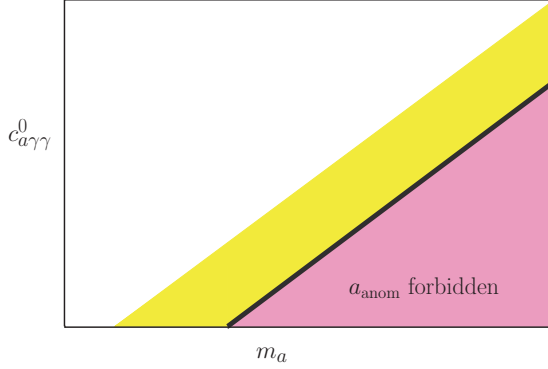


Fig. 6.15. A schematic view on $c_{a\gamma\gamma}^0$ vs. m_{axion} in string compactification. The thick line is for $c_{a\gamma\gamma}^0 = \frac{8}{3}$; the lavender part is forbidden if $U(1)_{\text{anom}}$ is the PQ symmetry, and the yellow band is the region to be looked for. In this scheme, the experimental bounds are shown in Fig. 9.11.

M_{GUT} if they are present. Therefore, we can allow the yellow band, but forbid the region of lavender color. If the PQ symmetry is approximate [76], then the lavender part is also possible.

“Invisible” axion scale from string

It is of utmost importance to bring the axion scale down to the intermediate scale which is the allowed axion window around $f_a \sim 10^{11}$ GeV in Fig. 9.11. In fact, it is possible to bring down the axion scale in string compactifications in case there is an anomalous $U(1)$. It is similar to the 't Hooft mechanism discussed in Section 4.4.4 in the standard spontaneous symmetry breaking. Here, the global direction is the MI axion and the gauge direction is the anomalous $U(1)$ gauge symmetry which is a subgroup of $E_8 \times E_8$ [79]. String theory written in 10D is anomaly-free. But, the point particle limit of the string theory seems to have an anomaly. In fact, Green and Schwarz found that there is a ten-dimensional (10D) term written in terms of the antisymmetric tensor field B_{MN} and $E_8 \times E_8$ gauge field strengths F_{MN} , and the inconsistency goes away [67]. The result is that the 10D point particle limit is anomaly-free. If a compactification of 10D string seems to lead a $U(1)$ gauge anomaly, then this GS term gives mass to the anomalous $U(1)$ gauge boson and there is no such gauge symmetry below this anomalous $U(1)$ gauge boson mass scale. But, there remains the global symmetry, which is the 't Hooft mechanism realized in the string compactification [72]. This global symmetry can be broken at the intermediate scale via the usual spontaneous symmetry breaking by the VEV, $\langle \phi \rangle$, of the global charge carrying scalar field ϕ .

Axions from string compactification will be discussed in more detail in Section 6.5.1.

6.4. Axions in astroparticle physics

There are two key parameters in the QCD axion models. One is the decay constant f_a and the other is the axion domain wall number N_{DW} . For $m_a \lesssim 23$ keV, Solar axions live long enough to reach at Earth. In addition, the “invisible” axion with mass smaller than ~ 24 eV could have survived until now. For this mass range, axions interact very weakly and can affect the evolutions of the Universe by f_a and N_{DW} and stars by f_a . In this section, we discuss briefly on the energy lost in stars by axion emission and on the energy density in the Universe contributed by cosmic axions. In Section 6.4.3, we will discuss the inflationary axion. The cosmological domain wall problem was discussed in Section 5.3 and related theories will be discussed more in Section 6.4.4.

Axion lifetime

Given $c_{a\gamma\gamma}$, the lifetime of axion is given by [37]

$$\tau(a \rightarrow 2\gamma) = \frac{2^8 \pi^3}{c_{a\gamma\gamma}^2 \alpha^2} \frac{f_a^2}{m_a^5} \simeq \frac{0.8 \times 10^7 t_U}{c_{a\gamma\gamma}^2} \left(\frac{\text{eV}}{m_a} \right)^3, \quad (6.140)$$

where $Z = 0.5$ is used and $t_U = 4.35 \times 10^{17}$ s is the age of the Universe. So, the lifetime is larger than t_U for $m_a \lesssim 24$ eV.

6.4.1. Axion–matter coupling and stellar axions

The axion coupling with the SM leptons is negligible in the KSVZ model. Their coupling arises at the one loop level and are about 10^{-4} level to that of the DFSZ model. Therefore, the astrophysical effects from $ae\bar{e}$ coupling are important in the DFSZ models. At high energy, the useful term is

$$\mathcal{L}_{ae\bar{e}} = c_1 \frac{\partial_\mu a}{f_a} \bar{e} \gamma^\mu \gamma_5 e, \quad c_1 = \mp \frac{\sin^2 \beta}{2N_{\text{DW}}} = \mp \frac{\sin^2 \beta}{6}, \quad (6.141)$$

where $\tan \beta = \langle H_u^0 \rangle / \langle H_d^0 \rangle$.

For the nucleon coupling, however, both the KSVZ and DFSZ couplings are important. Of course, the DFSZ couplings with light quarks are present as c_1 and c_2 terms of Eqs. (6.80) and (6.122). The KSVZ axions interact with gluons by the c_3 term and its interactions with light quarks can be significant. In Ref. [37], the axion–quark couplings are given as the $\bar{c}_1(\partial_\mu a)$ coupling to quarks $\bar{q} \gamma^\mu \gamma_5 q$ is related to $\bar{c}_2$ by $\bar{c}_1 = \frac{1}{2} \bar{c}_2$ for the KSVZ and $\bar{c}_1^{u,d} = \frac{1}{2} \bar{c}_2^{u,d} - \frac{1}{2}(|v_{d,u}|^2/v_{ew}^2)$ for the DFSZ. The c_1 couplings are the dominant ones in high energy axion interactions. For high energy axions, we summarize the results given in Eqs. (61) and (62) of Ref. [37] in general

case for contributions of one heavy quark and N_g families of light quarks,

$$\bar{c}_1^u = \frac{1}{2(1+Z)}(1^{\text{KSVZ}} \pm N_g^{\text{DFSZ}}) \mp \frac{v_d^2}{2v_{ew}^2} \delta_{H_u}, \quad (6.142)$$

$$\bar{c}_1^d = \frac{Z}{2(1+Z)}(1^{\text{KSVZ}} \pm N_g^{\text{DFSZ}}) \mp \frac{v_u^2}{2v_{ew}^2} \delta_{H_d}. \quad (6.143)$$

For the KSVZ axion models, we neglect N_g^{DFSZ} , and for the DFSZ axion models, we neglect 1^{KSVZ} . Here, δ_{H_u} and δ_{H_d} are the PQ quantum numbers of $H_{u,d}$ chosen as 0 for the KSVZ and +1 for the DFSZ of the above equations. Then, the nucleon couplings are given by [80]

$$\begin{aligned} C_{app} &= \bar{c}_1^u F + \frac{\bar{c}_1^u - 2\bar{c}_1^d}{3} D + \frac{\bar{c}_1^u + \bar{c}_1^d}{6} S \\ &= \left(-\frac{1}{6} - \frac{1}{2}s_\beta^2\right) F + \left(\frac{1}{2} + \frac{1}{2}s_\beta^2\right) D + \left(-\frac{1}{12} - \frac{1}{6}s_\beta^2\right) S, \end{aligned} \quad (6.144)$$

$$\begin{aligned} C_{ann} &= \bar{c}_1^d F + \frac{\bar{c}_1^d - 2\bar{c}_1^u}{3} D + \frac{\bar{c}_1^u + \bar{c}_1^d}{6} S \\ &= \left(-\frac{1}{3} - \frac{1}{2}s_\beta^2\right) F + \frac{1}{6}s_\beta^2 D + \left(-\frac{1}{12} - \frac{1}{6}s_\beta^2\right) S, \end{aligned} \quad (6.145)$$

where $F = 0.47$, $D = 0.81$, and $S \simeq 0.13 (\pm 0.2)$ are used for the nucleon parameters. The above nucleon coupling for the $Q_{\text{em}} = 0$ KSVZ model was used to estimate the lower bound of f_a [80]. The astrophysical bound from SN1987A is $f_a \geq 10^9$ GeV [81].

6.4.2. Axions in the cosmos

Cosmological energy density

As discussed in Section 6.1, BCM can behave as CDM if the potential is sufficiently flat. In Fig. 6.1, the vacuum denoted as the red bullet stays there if the Hubble parameter is larger than the oscillation rate of the BCM.

During the inflation, a sufficiently light scalar field becomes spatially homogeneous and its value is selected stochastically. After the inflation, the Hubble parameter decreases as the Universe expands. For the cosine potential of axion, if the Hubble parameter passes the bottleneck period discussed in Section 6.1, for the Hubble parameter somewhat smaller than the axion mass, the classical axion field $\langle a \rangle$ starts to roll down. In the hydrodynamic description, this collective motion of oscillation works as CDM in the evolution of the Universe. If the interaction is small enough to maintain a simultaneous collective motion until the MD era, it can be a part of the present matter energy density of the Universe. In this way, the “invisible” axion becomes CDM and can be collective and even coherent [11]

until now. In this section, we estimate the cosmological energy density of axions, following [7]. A recent estimate was given in [120].

The inflation freezes all fields whose masses are smaller than the Hubble parameter at that time. It also flattens the fluctuation of the field. On the other hand, scalar fields like that of the axion obtain quantum fluctuations during the inflation. These fluctuations have an important effect on CMB anisotropies. Just after the inflation, the sufficiently light fields remain homogeneous with a certain value that is determined stochastically. The QCD axion belongs to this class, and the field value is assumed to be $\langle a_1 \rangle = f_a \theta_1$. Its fluctuation will be discussed in Section 6.4.3. At the end of inflation, the Universe is reheated by some processes of inflaton decay. Since the axion is very weakly interacting, the reheated radiation of the early Universe cannot destroy the collectiveness of axions. As the Universe cools down, the Hubble friction can no longer be the dominant term and the axion field starts rolling down the potential hill and continues to oscillate. Since the Hubble parameter becomes smaller and smaller than the axion mass, or the oscillating period of the axion is smaller than the Hubble time, its energy and pressure can be described by time averages during each oscillation. In the case of the harmonic potential, the effective pressure is zero and the axion field acts like CDM in the evolving Universe. But, as discussed analytically in Section 6.1, the bottleneck to the cosine potential makes the Universe to cool down further to obtain the axion oscillation commencement angle $\theta_2 < \theta_1$. Moreover, if the axion maintains the collectiveness until the MD epoch, it can contribute to the present CDM energy density. During MD epoch until recently when the CDM density is overcome by the DE, the CDM density in the comoving volume remains constant, and the current CDM density is calculated. Comparing the resulting axion energy fraction Ω_a , we obtain the upper bound on f_a .

Since the axion mass depends on the temperature during the QCD phase transition [8, 82], the comoving energy density conservation alone does not work in estimating the axion relic density. However, the adiabatic theorem says that as long as the adiabatic conditions $H, \dot{m}_a/m_a \ll m_a$ hold, we can find the adiabatic invariant I . For the harmonic potential, the invariant is the comoving axion number density,

$$I = \frac{R^3 \rho_a(T)}{m_a(T)}. \quad (6.146)$$

Since the cosine potential does not guarantee the number eigenstate of the comoving volume, the interpretation as the number density does not work in general.

Let us parameterize the QCD instanton size integration at $T = T_{\text{GeV}}$ GeV near 1 GeV (from 700 MeV to 1.3 GeV) as [7, 82]

$$V(\theta) = -C(T) \cos(\theta), \quad \theta = \frac{a}{f_a}, \quad (6.147)$$

where

$$C(T) \equiv m^2(T)f_a^2 = \alpha_{\text{inst}} \text{GeV}^4 T_{\text{GeV}}^{-n}. \quad (6.148)$$

The temperature T_1 is calculated by $3H \simeq m_a$, using the relativistic degrees $g_* = 61.75$ at 1 GeV ($u, d, s, e, \mu, 3\nu, 3\bar{\nu}, \gamma$, and eight gluons) as

$$T_1 = \begin{cases} 1.229 \left(\frac{f_a}{10^{11} \text{GeV}} \right)^{-0.182} \text{GeV}, & \text{for } \Lambda_{\text{QCD}} = 320 \text{ MeV}, \\ 1.399 \left(\frac{f_a}{10^{11} \text{GeV}} \right)^{-0.184} \text{GeV}, & \text{for } \Lambda_{\text{QCD}} = 380 \text{ MeV}, \\ 1.512 \left(\frac{f_a}{10^{11} \text{GeV}} \right)^{-0.185} \text{GeV}, & \text{for } \Lambda_{\text{QCD}} = 440 \text{ MeV}, \end{cases} \quad (6.149)$$

where $n = 6.967, 6.878, 6.789$ are taken for $\Lambda_{\text{QCD}} = 320, 380, 440$ MeV, respectively. Note that the exponents, $-0.182 \sim -0.185$, are considered to be a constant. This constant may be taken as $-\frac{3}{16}$ instead of $-\frac{1}{6}$ used in most axion references.

Turner considered the anharmonic effect on the axion CDM energy density [61, 83, 84]. Later, Lyth presented an extensive study on this issue [62]. We follow the discussion presented in [7]. In the early epoch after the classical axion field starts to roll down, the axion number is not conserved because of the nonnegligible anharmonic terms. Physically, the introduction of the anharmonic terms means axion number changing interactions so that the axion number conservation is not guaranteed in the initial stage of rolling down. But, we can use the adiabatic invariant to treat this anharmonic effect. The axion field satisfies $\ddot{\theta} + 3H\dot{\theta} + \mathcal{V}' = 0$ with $\theta = a/f_a$, $\mathcal{V} = V/f_a^2$, and $\mathcal{V}' = d\mathcal{V}/d\theta$. This equation can be derived from the Lagrangian

$$L = R^3(f_a^2\dot{\theta}^2 - V(\theta)), \quad \text{with } V(\theta) = m_a^2 f_a^2 (1 - \cos \theta). \quad (6.150)$$

Here, we treat R and m_a as time-varying parameters. Under the adiabatic condition, $H, \dot{m}_a/m_a \ll m_a$, we have the adiabatically invariant quantity [85]:

$$I = \frac{1}{2\pi} \oint p dq, \quad \text{with } q = \theta, \quad p = R^3 \dot{\theta}. \quad (6.151)$$

Thus, we derive an invariant quantity of the axion oscillation as

$$R^3 m_a \bar{\theta}^2 f_1(\bar{\theta}) = \text{constant}, \quad (6.152)$$

where

$$f_1(\bar{\theta}) = \frac{2\sqrt{2}}{\pi\bar{\theta}^2} \int_{-\bar{\theta}}^{+\bar{\theta}} \sqrt{\cos \theta' - \cos \bar{\theta}} d\theta'. \quad (6.153)$$

The same form was also obtained in [62]. This effect of anharmonic term is in fact equivalent to the study of the bottleneck period discussed in Section 6.1. In Eq. (6.8), actually m_0 is a function of temperature, which is taken into account

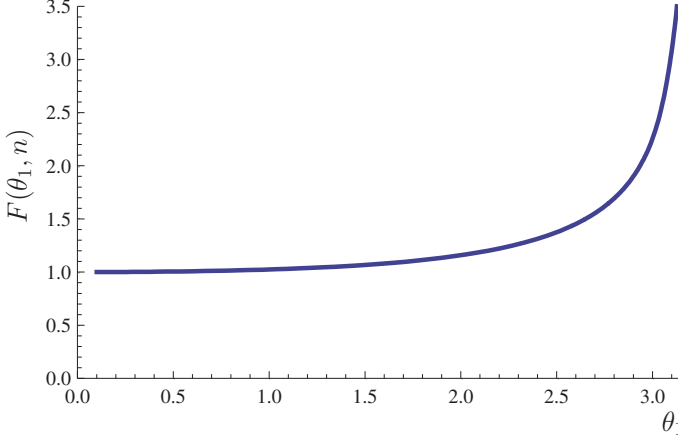


Fig. 6.16. The $\Omega_a = 1$ region in the $f_a - \theta_1$ plane [7].

in [7]. The axion energy density, using the new numbers for the current quark masses and including the above anharmonic effect and QCD phase transition effect [7], is estimated as

$$\rho_a(T_\gamma^{\text{now}}) \simeq 1.449 \cdot 10^{-12} \left(\frac{f_a}{10^{11} \text{ GeV}} \right) \left(\frac{\text{GeV}}{T_1} \right) \frac{\theta_1^2}{\gamma} F(\theta_1, n) [\text{eV}]^4, \quad (6.154)$$

where we used $g_{*s}(\text{present}) = 3.91$, $m_u/m_d = 0.5$, $m_{\pi^0} = 135.5 \text{ MeV}$, and $f_\pi = 93 \text{ MeV}$. $F(\theta_1, n) \simeq F(\theta_1)$ is the anharmonic correction given in Eq. (6.153), presented in Fig. 6.16, and γ is the entropy increase ratio during the quark–hadron phase transition. Since $\rho_c \simeq 0.81 \times 10^{-10} h^2 [\text{eV}]^4$, the energy fraction of CDM axion is, with the central value of the Planck cosmological parameter data on $h = 0.6731 \pm 0.0096$ [86],¹¹

$$\Omega_a = P(\Lambda_{\text{QCD}}) \left(\frac{\theta_1^2 F(\theta_1)}{\gamma} \right) \left(\frac{0.673}{h} \right)^2 \left(\frac{f_a}{10^{11} \text{ GeV}} \right)^{19/16}, \quad (6.155)$$

where

$$P(\Lambda_{\text{QCD}}) = \begin{cases} 0.317, & \text{for } \Lambda_{\text{QCD}} = 320 \text{ MeV}, \\ 0.280, & \text{for } \Lambda_{\text{QCD}} = 380 \text{ MeV}, \\ 0.251, & \text{for } \Lambda_{\text{QCD}} = 440 \text{ MeV}. \end{cases} \quad (6.156)$$

From $\Omega_{\text{CDM}} h^2 = 0.1197 \pm 0.0022$ [86], we obtain the bound $f_a \approx 3.4 \times 10^{11} \text{ GeV}$ for $\theta_1^2 = \gamma/F(\theta_1)$. For $\theta_1/\sqrt{\gamma} < 0.15$, $f_a \geq 10^{13} \text{ GeV}$ is allowed. The study in Ref. [7] used the QCD phase transition calculated with a bag model [121]. There is a new study based on the QCD phase transition by bubble formation in QFT.

¹¹It is a bit smaller than the WMAP data [87].

Axion window

The above cosmological and astrophysical effects narrowed down the allowed axion mass range in the region 10^{-3} – 10^{-5} eV, i.e., in the axion window of f_a ,

$$10^9 \text{ GeV} \lesssim f_a \lesssim 10^{11} \text{ GeV}. \quad (6.157)$$

Bose–Einstein condensation

In Section 6.1, a possibility for Bose–Einstein condensation of axions was discussed. It happens, if so, around the cosmic temperature near 500 eV. Its possible effects in the evolution of the Universe was categorized by case A and case B. In case A, thermal contacts are established before $\rho_{\text{matter}} = \rho_{\text{radiation}}$ between baryons and low momentum modes of axions. In case B, thermal equilibrium is reached before $\rho_{\text{matter}} = \rho_{\text{radiation}}$ between baryons, low momentum modes of axions, and photons. For case A, the cosmic evolution is the standard one we discussed above. For case B, expression of $\rho_{\text{radiation}}$ is effectively changed to [11, 88]

$$\rho_{\text{radiation}} = \rho_\gamma \left[1 + N_{\text{eff}} \frac{7}{8} \left(\frac{11}{4} \right)^{4/3} \right]. \quad (6.158)$$

Interpreting radiation as neutrinos, and condensed low momentum axions and condensed photons, N_{eff} is estimated as 6.77 [11]. Thus, case B seems to be unrealized [122].

6.4.3. Inflation with axion

During inflation, one takes into account massless bosons whose quantum fluctuation scales can be as large as the horizon scale. As discussed in Section 6.1, the classical QCD axion derives its mass when the temperature of the Universe falls below $T_2 < 1$ GeV. If the axion is a composite particle [89, 90], the axion degree is created below the symmetry breaking scale f_a where the non-Abelian force confines and the PQ symmetry is broken. Thus, for $T_{\text{reh}} > f_a$, it is meaningless to talk about a massless axion. But, if axion is a fundamental degree, axion is present all the time during the Universe evolution. In this case, the PQ symmetry breaking scale f_a is important at all scales in estimating its interaction effects, especially compared to the Hubble expansion rate H_I at the end of inflation. Thus, the axion phenomenology has another important H_I dependence.

Consider a fundamental degree axion. If f_a is smaller than H_I , one usually considers that topological defects of the axion vacuum such as axionic strings and domain walls are inflated away and that the inflation patch within which the horizon is embedded has the same misalignment angle θ_1 . If f_a is larger than H_I , one takes into account axionic topological defects and axion fluctuations also during inflation. Their imprints at H_I will become observable quantities at present. As shown in

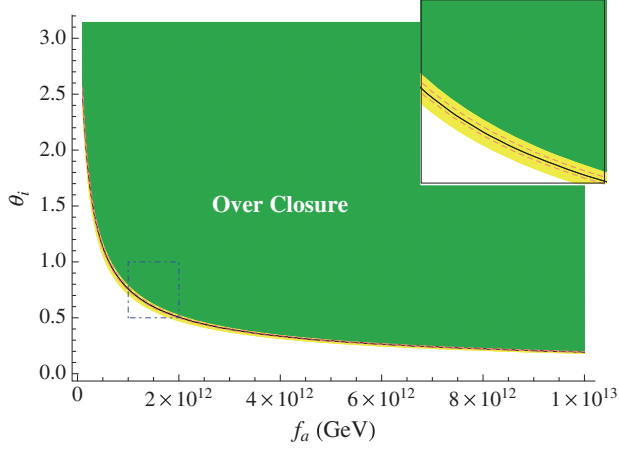
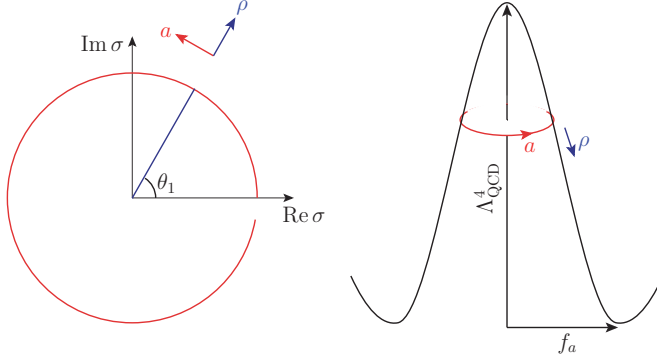


Fig. 6.17. The $\Omega_a < 1$ region (white) in the f_a – θ_1 plane [7].

Eq. (6.155), f_a (or the axion mass) is the key quantity obtaining the axion fraction Ω_a in the cosmic energy density, together with the misalignment angle θ_1 , as shown in Fig. 6.17 [7]. Pi considered inflation with the QCD axion field and argued for raising the bound on f_a to a GUT scale by fine-tuning of θ_1 at $O(10^{-3})$ [74]. During inflation, any patch with a value near θ_1 is expanding and the θ_1 region as small as $\sim 10^{-3}$ can become our Universe. Probabilistically, it is unlikely, but with f_a at the GUT scale, only regions with $\theta_1 \lesssim 10^{-3}$ could have evolved to a long-lived Universe for life forms to be hospitable. It is based on the “anthropic principle” [91]. This anthropic window has been studied in [75]. Embedding the QCD axion in the phase of a complex scalar field σ , $\sigma = \frac{1}{\sqrt{2}}(f_a + \rho)e^{ia/f_a}$, we must consider two real fields ρ and a . Both fields must be considered during inflation in the hilltop potential of axion field as shown in Fig. 6.18 [84, 92, 93]. Since f_a is large, it is almost flat in the ρ direction which is the inflaton. In the a direction, the height of V does not change. After θ_1 (or $\langle a \rangle$) is chosen, we can consider some neighborhood of θ_1 , with $\delta\theta_1$ variance. Even though $\delta\theta_1$ is considered, V does not change and this direction is considered *isocurvature* perturbation. Inflation in this direction is also called isothermal inflation. In this axion inflation, there are two modes: the adiabatic mode ρ and the isothermal mode a .

If vacuum energy is of order GUT scale M_{GUT}^4 , the Hubble parameter at that scale is of order $M_{\text{GUT}}^2/M_{\text{P}} \sim 10^{-2}M_{\text{GUT}} \sim 2 \times 10^{14}$ GeV. Since the recent observations indicate that the GUT scale inflation is not ruled out [94], it is useful to consider this small region of the misalignment angle θ_1 during inflation with the QCD axion. Let us introduce an inflaton which is not ρ of the QCD axion model such that $V = V_I + V_{\text{QCD}}$ with $V_I \gg V_{\text{QCD}}$. This scalar amplitude of perturbations generated during inflation is given by

$$\mathcal{A}_s = \frac{1}{2\epsilon} \left(\frac{H_I}{2\pi M_{\text{P}}} \right)^2, \quad (6.159)$$

Fig. 6.18. Two directions of σ in V [84].

where the slow-roll parameter ϵ and H_I are derived from V_I . For the slow-roll inflation, ϵ must be small,

$$\epsilon \simeq \frac{M_{\text{P}}^2}{2} \left(\frac{V'_I}{V} \right)^2 \ll 1. \quad (6.160)$$

Fluctuations from the zero-point fluctuations of the classical graviton field has the amplitude

$$\mathcal{A}_T = \frac{1}{8} \left(\frac{H_I}{2\pi M_{\text{P}}} \right)^2. \quad (6.161)$$

Thus, the ratio of the tensor to scalar in inflationary models is

$$r = \frac{\mathcal{A}_T}{\mathcal{A}_s} = 16\epsilon. \quad (6.162)$$

After the initial confusion on the magnitude on r [94], the current upper limit is given by $r \lesssim 0.11$ [95].

The relic density is determined by spatially averaged misalignment angle [62, 96–98],

$$\langle \theta_1^2 \rangle = \delta\theta_1^2 + (H_I/2\sqrt{2}\pi f_a)^2, \quad (6.163)$$

where $\delta\theta_1$ is the variance or dispersion of θ near θ_1 . In addition to (6.163), we must also consider fluctuations in the geometry. The isocurvature perturbation is concretely given in terms of Fourier components in [62]. In the de Sitter space, all minimally coupled massless fields have the Hawking radiation [99] given by temperature $H_I/2\pi$ where H_I is the Hubble scale in the de Sitter phase. Variance of these quantum fluctuations is $H_I/2\sqrt{2}\pi$. Hawking radiation will generate fluctuations of order H_I for all massless fields. After inflation, we have the fluctuations during inflation imprinted “historically” at the end of inflation. Therefore, we always consider the second term of Eq. (6.163). But, when $\text{U}(1)_{\text{PQ}}$ is broken before or during

inflation, $f_a > H_I/2\sqrt{2}\pi$, even if the axion is a fundamental massless field, the practical relevance for the first term in Eq. (6.163) is unimportant because the entire present Universe lies within one horizon. Using Eq. (6.163), in view of [94], the values based on Refs. [100, 101] are

$$\begin{aligned}\Omega_a &= P(\Lambda_{\text{QCD}}) \left(\frac{\theta_1^2 F(\theta_1)}{\gamma} \right) \left(\frac{0.673}{h} \right)^2 \left(\frac{f_a}{10^{11} \text{ GeV}} \right)^{19/16}, \text{ for } f_a \lesssim \hat{f}_a, \\ \Omega_a h^2 &= 0.0051 \langle \theta_1^2 f(\theta_1) \rangle (f_{a,\text{GeV}})^{3/2}, \text{ for } f_a \gtrsim \hat{f}_a,\end{aligned}\tag{6.164}$$

where $\hat{f}_a \simeq 0.99 \times 10^{17} \text{ GeV}$ [101] and $P(\Lambda_{\text{QCD}})$ is given in (6.156). The bound $\hat{f}_a$ is given at the end of quark-hadron phase transition. At $T < 100 \text{ MeV}$, the transition is considered to be finished, and using $g_* = \frac{25}{2}$ from $\gamma, e^\pm$ and 3ν allows the temperature-independent axion mass below $\hat{f}_a$, and $3H \lesssim m_a$ gives the above fraction.

Including the anthropic region, we can consider f_a below and above H_I ,

Scenario A: PQ symmetry breaking after inflation, $H_I > f_a$,

Scenario B: PQ symmetry breaking before or during inflation, $f_a \gtrsim H_I$.

In scenario A, θ_1 is not uniform over a Hubble volume, so θ_1^2 is averaged over its possible values and is given as $\langle \theta_1^2 F(\theta_1) \rangle = 2.67\pi^2/3$ [102]. From Eq. (6.155), we obtain for $\Lambda = 380 \text{ MeV}$,

$$\Omega_a h^2 = \frac{1.11}{\gamma} \left(\frac{f_a}{10^{11} \text{ GeV}} \right)^{19/16}.\tag{6.165}$$

To obtain $\Omega_a h^2 \simeq 0.1197$, we obtain $f_a \sim 1.7 \times 10^{10} \text{ GeV}$, predicting $\sim m_a \simeq 10^{-3} \text{ eV}$, where we have not included the production of axion strings and domain walls. We have not included $\delta\theta_1^2$ of Eq. (6.163) which is also of the same order. In scenario B, the first term in Eq. (6.163) can be neglected. But the second term is present, and the limit $V_I \lesssim M_{\text{GUT}}^4$ gives $H_I < 10^{14} \text{ GeV}$. The excluded region from this $H_I > 10^{14} \text{ GeV}$ is shown as the top skyblue box in Fig. 6.19. For the anthropic values of $\theta_1 \leq 0.1$, the allowed H_I values are shown as vertical lines in Fig. 6.19. In this figure, the cosmic string contribution [16] to the energy density is also taken into account. The interesting region for high-scale inflation is the white in the upper left region.

The horizon crossing condition of the scale k^{-1} is

$$k^{-1}R(t) = H^{-1}(t).\tag{6.166}$$

Since we need an inflation exponentiating the scale factor by $R \gtrsim 10^{27}$, the above equation gives for δ at $T_1 \lesssim 1 \text{ GeV}$, $k = RH > 10^{-8} \sqrt{g_*/3} T_1^2 / \text{GeV}$. In Fig. 6.20, δ is given at this temperature. At T_1 , the dispersion $\delta\rho_a/\rho_a$ is much smaller than

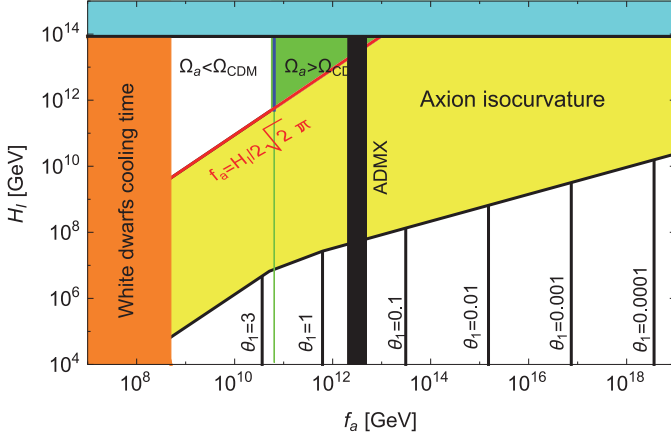


Fig. 6.19. A schematic view [101] of possible regions from isocurvature perturbations in the H_I vs. f_a plane. The white region is allowed.

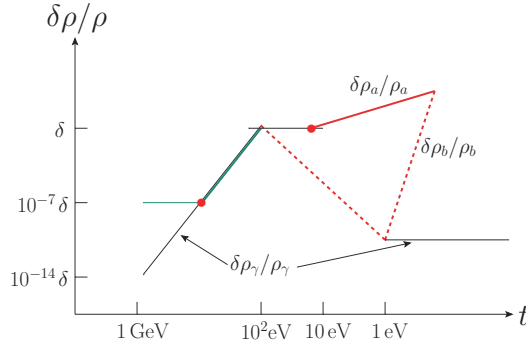


Fig. 6.20. Sketch of the time evolution of galactic scale axion density fluctuations after inflation [93].

δ , which is marked as $10^{-14}\delta$ for an illustration. After inflation, if θ_1 and f_a are in the allowed region of Fig. 6.19, the time evolution of galactic scale axion density fluctuations is sketched here, following Ref. [93]. Since $\rho_a \propto T^3$ and $\rho_\gamma \propto T^4$, we have, for small fluctuations,

$$\left. \frac{\delta \rho_a}{\rho_a} \right|_{T_1} \simeq \frac{3}{4} \left. \frac{\delta \rho_\gamma}{\rho_\gamma} \right|_{T_1}. \quad (6.167)$$

Equating Eq. (6.154) at temperature T with the radiation energy $(\pi^2/30)g_*T^4$, we obtain the radiation–axion equality temperature,

$$T_{\text{eq}}^a \simeq 0.358 \left(\frac{f_a}{10^{11} \text{ GeV}} \right) \left(\frac{\text{GeV}}{T_1} \right) \left(\frac{\theta_1 F(\theta_1)}{\gamma g_*} \right) [\text{eV}]. \quad (6.168)$$

If $f_a \sim 10^{12}$ GeV, T_{eq}^a can be of order 10 eV. With the current bound on f_a , T_{eq}^a seems to be less than 10 eV. Usually, $T_{\text{eq}} \simeq 100$ eV is taken, considering multi-components of CDM. After T_{eq}^a is passed, $\delta\rho_a/\rho_a$ grows as shown with the red line. During this period, ratio of the radiation fluctuation to the axion fluctuation decreases for some time until the end of Silk damping. After the Silk damping, the baryon fluctuation grows, following the CDM fluctuations as shown with the red dashed lines.

6.4.4. Domain wall problem

Now, the Goldstone boson direction in Fig. 5.8 can be the gauge group direction or a Goldstone boson direction in some spontaneously broken continuous symmetries [103]. Lazarides and Shafi noted the former possibility in GUT models [104]. It depends on the center of extended GUT groups [47]. In this case, one should not worry about the domain wall problem at all, except the cosmological evolution [105, 106]. The discrete element commuting with all elements of the group is called the center of the group. The centers of non-Abelian groups are [107]

$$\begin{aligned}
 \text{SU}(N): \mathbf{Z}_N, \quad N \geq 2, \\
 \text{SO}(2\ell + 1): \mathbf{Z}_2, \quad \ell \geq 2, \\
 \text{SO}(4\ell + 2): \mathbf{Z}_4, \quad \ell \geq 2, \\
 \text{Sp}(2n): \mathbf{Z}_2, \quad n \geq 2, \\
 \text{E}_6: \mathbf{Z}_3, \\
 \text{E}_7: \mathbf{Z}_2, \\
 \text{E}_8, \text{F}_4, \text{G}_2: \text{trivial}.
 \end{aligned} \tag{6.169}$$

For real adjoint representations, the hypothetical discrete group elements commute. So, the center is checked for complex representations of the discrete group which allow nontrivial phase rotations. Some examples are as follows.

Example 6.4 (Centers). An adjoint representation for a scalar field is real. So, if the adjoint representation is the fundamental representation, the center of the group is trivial. Therefore, to see a nontrivial case, let us consider two points of some complex operator.

For E_6 , the complexity of **27** can be studied with the complexity under its subgroup $\text{SU}(3)^3$, $\mathbf{27} \equiv \Phi = (\mathbf{3}, \bar{\mathbf{3}}, \mathbf{1}) + (\bar{\mathbf{3}}, \mathbf{1}, \mathbf{3}) + (\mathbf{1}, \mathbf{3}, \bar{\mathbf{3}})$. Thus, a gauge group invariant effective operator Φ^3 can be studied where the complexity is abolished at some field points. They are at the points of Φ at $\propto e^{i2\pi \frac{n}{3}}$ with $n = 0, 1, 2$. These three different field points of Φ define the center of E_6 as $\mathbf{Z}_3$.

For a fundamental representation $\phi^\alpha \equiv \mathbf{N}$ of $\text{SU}(N)$, a gauge group invariant effective operator $\epsilon_{\alpha_1 \alpha_2 \dots \alpha_N} \phi^{\alpha_1} \phi^{\alpha_2} \dots \phi^{\alpha_N}$ can be considered. It is not complex at the points of ϕ at $\propto e^{i2\pi \frac{n}{N}}$ with $n = 0, 1, 2, \dots, N-1$. These N different field points of ϕ define the center of $\text{SU}(N)$ as $\mathbf{Z}_N$.

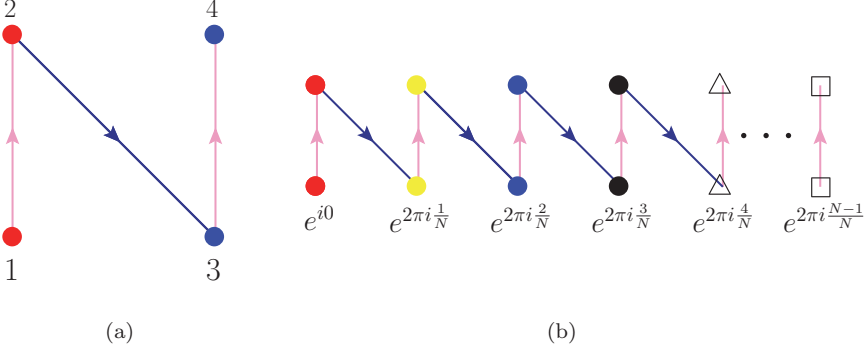


Fig. 6.21. Gauge transformations (blue arrows) connecting the centers: (a) $SU(2)$ and (b) $SU(N)$.

For a spinor representation $\Psi \equiv \mathbf{16}$ of $SO(10)$, a gauge group invariant effective operator Ψ^4 can be considered. It is not complex at the points of Ψ at $\propto e^{i2\pi \frac{n}{4}}$ with $n = 0, 1, 2, 4$. These four different field points of Ψ define the center of $SO(10)$ as $\mathbf{Z}_4$.

The above effective operators are gauge invariant and hence two points of the effective operators are connected by some gauge transformation.

Example 6.5 (Gauge transformation between centers of $SU(N)$). First consider $SU(2)$. The fundamental representation ϕ is

$$\phi = \begin{pmatrix} \phi_{\uparrow} \\ \phi_{\downarrow} \end{pmatrix}. \quad (6.170)$$

The gauge transformation operator by α in the $T_3 = \sigma_3/2$ direction is $e^{iT_3\alpha} = \cos \frac{\alpha}{2} \mathbf{1} + i \sin \frac{\alpha}{2} \sigma_3$. Thus, we obtain, for $\alpha = 2\pi = 4\pi \left(\frac{1}{2}\right)$,

$$\phi \rightarrow (\cos \pi \mathbf{1} + i \sin \pi \sigma_3) \begin{pmatrix} \phi_{\uparrow} \\ \phi_{\downarrow} \end{pmatrix} = - \begin{pmatrix} \phi_{\uparrow} \\ \phi_{\downarrow} \end{pmatrix} = e^{2\pi i \frac{1}{N}} \phi, \quad (6.171)$$

with $N = 2$. It is shown in Fig. 6.21(a). Points 1 and 2 are the identical points, so are Points 3 and 4. They are shown at separated points as in the cases of torus identification. The blue arrow is the gauge transformation with the generator T_3 .

Now, consider $SU(N)$ with the generator $F_{N^2-1} = \lambda_{N^2-1}/2$,

$$\tilde{\lambda}_{N^2-1} = \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & -(N-1) \end{pmatrix},$$

where $\lambda_{N^2-1} = \sqrt{2} \tilde{\lambda}_{N^2-1} / \sqrt{N^2 - N}$. Let Ψ be a fundamental representation of $SU(N)$. $e^{i\tilde{\lambda}_{N^2-1}\alpha}$ on Ψ is

$$\Psi \rightarrow \begin{pmatrix} e^{i\alpha} & 0 & \cdots & 0 & 0 \\ 0 & e^{i\alpha} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & e^{i\alpha} & 0 \\ 0 & 0 & \cdots & 0 & e^{-i(N-1)\alpha} \end{pmatrix} \Psi.$$

Choosing $\alpha = 2\pi/N$, we obtain $e^{i\tilde{\lambda}_{N^2-1}(2\pi/N)}$ on Ψ is

$$\Psi \rightarrow \begin{pmatrix} e^{2\pi i/N} & 0 & \cdots & 0 & 0 \\ 0 & e^{2\pi i/N} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & e^{2\pi i/N} & 0 \\ 0 & 0 & \cdots & 0 & e^{-2\pi i(N-1)/N} \end{pmatrix} \Psi = e^{2\pi i/N} \Psi. \quad (6.172)$$

Thus, we go from one vacuum to the next one, e.g., from the red bullet to the yellow bullet in Fig. 6.21(b). Continuing this gauge transformation, we identify all the N vacua of Fig. 6.21(b).

Even if the gauge group is spontaneously broken, this identification method is valid because the gauge transformation direction becomes the longitudinal direction of the broken gauge generator, i.e., it is a true Goldstone boson direction. The extended GUTs have been used in this way to make $N_{\text{DW}} = 1$ models [108].

6.5. Non-QCD axions

At low energy with the SM non-Abelian gauge fields, G_μ^a and W_μ^i , non-QCD axions are pseudoscalars, not coupling to the color anomaly,

$$\text{Non-QCD axions} \begin{cases} 1. \text{ no coupling to } \{G\tilde{G}\}, \\ 2. \text{ but may couple to } \{W\tilde{W}\}, \\ 3. \text{ or also no coupling to } \{W\tilde{W}\}, \\ 4. \text{ and coupling to } \{F_{\text{em}}\tilde{F}_{\text{em}}\}. \end{cases} \quad (6.173)$$

Phenomenologically, cases 2 and 3 are indistinguishable because $SU(2)_W$ does not confine and the instanton effect is negligible $\sim e^{-2\pi/\alpha_2}$. Case 4, if it is very light, corresponds to pseudoscalars called axion-like particles (ALPs) because the detection method in case 4 uses the same type of coupling $\{F_{\text{em}}\tilde{F}_{\text{em}}\}$ as for the detection of the QCD axion. Note, however, that “axion” is named for the pseudoscalar which

has the coupling to gluon anomaly, derived from the anomaly of the axial-vector current.¹²

6.5.1. Superstring axions

String theory, the most popular ultraviolet-completed theory, houses plenty of pseudoscalar particles. They come from the antisymmetric field B_{MN} [68] and matter representation [109]. They are called axions because their equations of motion imply their couplings to non-Abelian anomaly. The axion, arising in any compactification scheme from $B_{\mu\nu}$ ($\mu, \nu = 1, \dots, 4$), is the “MI axion”. The string axion, depending on the compactification scheme, is called “model-dependent (MD) axion”.

B_{MN} is a gauge field in higher dimensions, transforming covariantly under the gauge transformation as

$$B_{MN} \rightarrow B_{MN} + \partial_M \Lambda_N - \partial_N \Lambda_M, \quad (6.174)$$

where Λ_M are gauge potentials. In superstring theory, M runs over $1, 2, \dots, 10$, with $1, \dots, 4$ belonging to the four-dimensional (4D) Minkowski space. Its field strength is¹³

$$\begin{aligned} H_{MNP}^{(0)} &= \partial_M B_{NP} + \partial_N B_{PM} + \partial_P B_{MN} \\ &\quad - \partial_P B_{NM} - \partial_N B_{MP} - \partial_M B_{PN}, \end{aligned} \quad (6.175)$$

where the notation (0) will be explained below. Green and Schwarz found that the multi-index gauge field B_{MN} makes the theory anomaly-free by inserting the GS term [67],

$$\begin{aligned} S_0 &= \int d^{10}x \exp \left[-\frac{\kappa^{-2}}{2} \mathcal{R} - \frac{\kappa^{-2}}{\varphi^2} \partial_M \varphi \partial^M \varphi - \frac{1}{4g^2 \varphi} F_{MN} F^{MN} \right. \\ &\quad \left. - \frac{3\kappa^2}{2g^4 \varphi^2} H_{MNP} H^{MNP} \right], \end{aligned} \quad (6.176)$$

where φ is dilaton, and only bosonic couplings are shown. The canonical dimensions of φ , κ , and g are 0, -4 , and -3 , respectively. The canonical dimensions of H^{MNP} and B^{MN} are 3 and 2, respectively. Instead of $H_{MNP}^{(0)}$ of Eq. (6.175), Ref. [67] made

¹²F. Wilczek is frequently quoted for mentioning the “axion” detergent.

¹³The antisymmetric tensor $H_{[MNP]}$ is customarily denoted without the bracket, H_{MNP} .

the theory anomaly-free for $E_8 \times E_8'$ gauge group by defining the 3-form

$$H = dB + \frac{1}{30} \omega_{3Y_1}^0 + \frac{1}{30} \omega_{3Y_2}^0 - \omega_{3L}^0, \quad (6.177)$$

where the 3-form dB gives (6.175), and the Yang–Mills Chern–Simon 3-forms for $E_8 \times E_8'$ and Lorentz group are

$$\begin{aligned} \omega_{3Y_1}^0 &= \text{Tr} \left(A_1 F_1 - \frac{1}{3} A_1^3 \right), \quad \omega_{3Y_2}^0 = \text{Tr} \left(A_2 F_2 - \frac{1}{3} A_2^3 \right), \\ \omega_{3L}^0 &= \text{Tr} \left(\omega \mathcal{R} - \frac{1}{3} \omega^3 \right), \end{aligned} \quad (6.178)$$

where

$$\begin{aligned} B &= B_{MN} dx^M \wedge dx^N, \quad \omega = \omega_M dx^M, \\ \mathcal{R} &= d\omega + \omega^2, \quad d\omega_{3L}^0 = \text{Tr} \mathcal{R}^2. \end{aligned} \quad (6.179)$$

In 4D, B_{MN} gives only pseudoscalars. Thus, to write them as scalars explicitly, the gauge invariant form H_{MNP} of dimension 3 is used.

If M, N , and P are the Minkowski indices, $\mu, \nu, \rho = \{1, \dots, 4\}$, we can write the antisymmetric tensor as

$$H_{\mu\nu\rho} = M_{MI} \epsilon_{\mu\nu\rho\sigma} \partial^\sigma a_{MI}. \quad (6.180)$$

Since any compactification must obtain 4D Minkowski space, the above pseudoscalar is called the MI axion. Comparing the first and the last terms of (6.176), Ref. [69] obtained the decay constant

$$f_{MI} \simeq 10^{16} \text{ GeV}. \quad (6.181)$$

If only one among M, N , and P is the Minkowski indices, we can write the antisymmetric tensor as

$$H_{\mu MN} = M_{MD} \epsilon_{MN} \partial_\mu a_{MD}. \quad (6.182)$$

Thus, this axion depends on the compactification scheme, determining ϵ_{MN} [68, 69]. Also, in most cases, the decay constant is near the string scale [70].

The basis for calling H_{MNP} as axions is based on the coupling (6.177). Taking the 4-form from (6.177) for the gauge group $E_8 \times E_8'$ is

$$dH = \frac{1}{30} \text{Tr} \mathcal{F}_1^2 + \frac{1}{30} \text{Tr} \mathcal{F}_2^2 - \text{Tr} \mathcal{R}^2, \quad (6.183)$$

where 3-forms in (6.178) are used and the subscripts 1 and 2 refer to E_8 and E_8' ,

respectively. Thus, we have

$$\partial_\mu H_{\nu\rho\sigma} \propto \frac{1}{30} \{F_{1\mu\nu} \tilde{F}_1^{\mu\nu}\} + \frac{1}{30} \{F_{2\mu\nu} \tilde{F}_2^{\mu\nu}\}, \quad (6.184)$$

where the left-hand side is proportional to $\partial^2 a_{MI}$. Equation (6.184) is the equation of motion for a_{MI} and hence the interaction Lagrangian of the MI axion coupling is

$$\frac{a_{MI}}{f_{MI}} (\{F_{1\mu\nu} \tilde{F}_1^{\mu\nu}\} + \{F_{2\mu\nu} \tilde{F}_2^{\mu\nu}\}). \quad (6.185)$$

So, any non-Abelian anomaly and all U(1) gauge anomaly couple to the MI axion with the same coefficient. Here, f_{MI} is proportional to M_1 as shown in [69].

For the MD axion(s), some may couple to some non-Abelian anomaly, but some may not couple to any non-Abelian anomaly at all. They depend on the compactification scheme [69].

f_a in the axion window

Finally, we comment on how to generate f_a in the axion window (6.157) in string compactification [109]. As an example, consider the MI axion. If there is no anomalous U(1) gauge symmetry in string compactification, then the decay constant is of order 10^{16} GeV as discussed in [69]. However, if there is an anomalous U(1) gauge symmetry, the corresponding gauge boson obtains mass by absorbing the MI axion as its longitudinal degree. Then, below the mass scale of the anomalous U(1) gauge boson, there emerges a global U(1) symmetry with charges corresponding to those of the mother anomalous U(1) gauge symmetry [73, 110]. Thus, from the anomalous U(1) symmetry, the axion is in fact the matter axion not coming from $B_{\mu\nu}$ but from the phases of scalar singlets. Thus, f_a can be at the axion window of $10^9 - 10^{11}$ GeV. Even if there was no global symmetry in string theory, there results a global symmetry in the end, after compactification. This is the string realization of the 't Hooft mechanism discussed in Sections 4.4 and 6.3.6.

There have been many discussions on the Fayet-Iliopoulos (FI) D -term for $U(1)_{\text{anom}}$ gauge symmetry at the GUT scale. However, there is no gauged U(1) corresponding to the anomalous symmetry below the compactification scale. It is obvious for models with a hierarchy between the compactification scale and the GUT scale. If we consider the $U(1)_{\text{anom}}$ D -term, $\int d^4\theta \xi D$, the potential has a contribution, $\frac{1}{2} D^2$, with $D = -\xi - e_a \phi^* Q_a \phi$ where e_a is the $U(1)_{\text{anom}}$ gauge coupling. Our $U(1)_{\text{anom}}$ is derived from the orbifold compactification of the $E_8 \times E'_8$ heterotic string. After compactification of the six internal space, one can consider $M_4 \times K$ where M_4 is the Minkowski space and K is the internal space. In the compactification of $E_8 \times E'_8$ heterotic string, there appears only one anomalous U(1) if any such terms are present. If so, the corresponding gauge boson obtains mass by absorbing a_{MI} as discussed in Section 6.3.6. This is the argument from effective field theory.

In string loop calculation, it is reported that the FI D -term is generated at string two loop [123].

Even if we consider the FI term with a nonvanishing ξ , which can be applied to the case without the hierarchy between the compactification and GUT scales, we can consider the $\epsilon^{\mu\nu\rho\sigma} H_{\mu\nu\rho} \partial_\sigma a_{\text{MI}}$ term plus the D term [72],

$$\begin{aligned} & \frac{1}{2} \partial^\mu a_{\text{MI}} \partial_\mu a_{\text{MI}} + M_{\text{MI}} A_\mu \partial^\mu a_{\text{MI}} + \left| -\xi + e \sum_a \phi_a^* Q_a \phi_a \right|^2 \\ & + \left[|(\partial_\mu - ie A_\mu) \phi_1|^2 + \cdots \right] = (M_{\text{MI}} \partial^\mu a_{\text{MI}} - e V_1 \partial^\mu a_1) A_\mu + \cdots, \end{aligned} \quad (6.186)$$

where ϕ_a are assumed to carry only the anomalous charge for this purpose, not carrying any nonanomalous charges, including Y . Let one ϕ_a , say ϕ_1 develops a VEV, V_1 , by minimizing the FI term. Here, two phase fields, a_{MI} and a_1 [= the phase of $\phi_1 = (V_1 + \rho_1) e^{ia_1/V_1} / \sqrt{2}$], are considered and only one Goldstone boson is absorbed to A_μ ,

$$\sqrt{M_{\text{MI}}^2 + e^2 V_1^2} (\cos \theta_G a_{\text{MI}} - \sin \theta_G a_1), \quad (6.187)$$

where $\tan \theta_G = e_a V_1 / M_{\text{MI}}$. The orthogonal Goldstone boson direction

$$a' = \cos \theta_G a_1 + \sin \theta_G a_{\text{MI}} \quad (6.188)$$

is surviving as a global direction below the scale $\sqrt{M_{\text{MI}}^2 + e_a^2 V_1^2}$. With this global symmetry, we can consider breaking other nonanomalous $U(1)$ gauge symmetries around the GUT scale, repeating the 't Hooft mechanism many times, we can obtain only one global symmetry to the axion window.

6.5.2. Axion-like particles

Some of these pseudoscalar particles behave like axions in that their couplings to photons are via the Primakoff coupling, $c_{a\gamma\gamma} \{F_{\text{em}} \tilde{F}_{\text{em}}\}$. If these particles are light, the only way to detect them is via the Primakoff interaction. Thus, the detection methods are identical to those of the QCD axion and hence are called axion-like particles (ALPs). The axion search experiments can be used for ALP detection also. Since an ALP mass is not related to the QCD anomaly, it is a free parameter. Their mass arises from the potential V of Fig. 6.13 (a) and from other non-Abelian anomaly such as $SU(2)$ of the SM and some from the hidden sector gauge group E'_8 .

6.5.3. Ultra-light axions

Recently, very very light axions have been considered for an effective cosmological constant (CC) and also to cure the cusp-core problems in the structure formation [19–22]. The former case with mass of order 10^{-33} eV and $f \sim 10^{19}$ GeV [111] can mimic the CC and hence can be called “CC axion (CCA)”. The second case with

mass of order 10^{-22} eV and $f \sim 10^{17}$ GeV is called ULA. For CCA to be realized theoretically, firstly there is no CCA- G - G anomaly with a non-Abelian gauge group G and second the definition of the global $U(1)_{\text{DE}}$ symmetry with the Planck scale decay constant is realized at a sufficiently high order such that its breaking by a potential term ΔV of Fig. 6.13 (a) is very very weak [112, 113].

It must be a non-QCD axion φ , and behaves as BCM [114]. A quantum fluctuation of the quantum field φ follows the same scenario, viz. Fig. 2.3, of entering into the inflationary period and re-entering into the horizon as the density perturbation $\delta\rho/\rho$ does. For the ULA, the re-entry time of the fluctuations was suggested, according to the model builders. If the re-entry has not occurred yet, it is CCA [111–113]. If the re-entry has occurred between “CDM density fixed” and “matter = radiation” in Figs. 1.3 and 2.3, it behaves like another DM candidate. For $m_\varphi \simeq 10^{-22}$ eV and $f_\varphi \simeq M_{\text{GUT}}$, the cusp-core and the dwarf galaxy problems can be understood [19, 20]. With an approximate discrete symmetry, this scenario can be realized with a very small ΔV of Fig. 6.13(a) [21]. Also, the $SU(2)$ force of the SM can provide this kind of ULA. Some astrophysical arguments are presented in Ref. [22].

6.5.4. Other scalar BCMs

The basic idea in any “scalar” collective motion for CDM is not much different from the case of axion CDM. To be specific, here we have discussed the axion case but with the proviso that one may replace the PQ scale f_a by some other effective mass scale in other bosonic cases. This decay constant scale of a scalar is model-dependent. For the case of dilaton, it can be taken as the Planck scale since the scale (i.e., the mass parameter) is defined by giving M_{P}^2 in front of the Ricci scalar $\mathcal{R}$.

For the dilaton BCM, it has to be oscillating now. Assuming $f \simeq M_{\text{P}}$, the explicit symmetry breaking scale for 10^{-22} eV mass is

$$\Delta V_{\text{dilation sym breaking}} \simeq (0.5 \text{ keV})^4. \quad (6.189)$$

Thus, dilaton for ultra-light scalar may be difficult to be realized since the electroweak symmetry breaking and the QCD chiral symmetry breaking may introduce a larger breaking scale.

6.6. Gravity effects

Gravity effects break most symmetries except gauge symmetries. We introduced it before. In this section, we consider discrete symmetries before applying it to the WIMPs in the next chapter. Since there does not exist a universally accepted quantum gravity theory at present, our discussion proceeds via a plausible aspects of gravity sector by topology change, i.e., in connection with wormholes and

black holes. These topology change can affect information stored in the visible Universe.

6.6.1. Spacetime manifolds

Let us consider first the case of four spacetime dimensions where information flows out of black holes. Here, we depict the situation for some flux lines going out from a black hole in Fig. 6.22(a). If they are magnetic flux lines, one can draw some physical argument. For the thrown out magnetic field not to be observable, it must satisfy the Dirac quantization condition on the magnetic charge g , $eg = \frac{1}{2} \cdot (\text{integer})$. If the flux lines are sufficiently shrinkable, the integral $\mathbf{B}$ -flux $= \int dx^\mu A_\mu$ shown as the red arrow via Stokes theorem must satisfy the quantization condition so that there is no hair of $\mathbf{B}$ field from the black hole. Now, let us consider a case where a unit magnetic charge is placed inside a black hole as in Fig. 6.22(b). If the black hole is well placed, one can observe its size as in Fig. 6.22(b). Thus, the $\mathbf{B}$ -flux from the magnetic monopole must be well defined at the radius of the black hole R_{BH} , i.e., the solid angle $\Delta\Omega$ corresponding to the monopole radius considered in Section 5.1 must be very small compared to R_{BH} . It can be quantified by

$$|\mathbf{B}| r^2 \Delta\Omega \ll 4\pi, \quad (6.190)$$

which can be rewritten in terms of the black hole radius R_{BH} as

$$|\mathbf{B}| R_{\text{BH}}^2 \left(\frac{r_{\text{unit}}^2}{R_{\text{BH}}^2} \right) \ll 1. \quad (6.191)$$

Expressing the magnetic charge in terms of electric charge e , at the radius R_{BH} , we have

$$\frac{1/e}{4\pi} \left(\frac{r_{\text{unit}}^2}{R_{\text{BH}}^2} \right) \ll 1. \quad (6.192)$$

This condition is satisfied for a sufficiently large R_{BH} , i.e., sufficiently massive black hole. If a black hole is not sufficiently massive, R_{BH} cannot be sufficiently large and the condition (6.192) cannot be satisfied. If the condition (6.192) is not satisfied, we cannot obtain a situation that the magnetic charge is quantized. Then, the black hole has the observable magnetic flux lines. To avoid this worrisome situation, Ref. [115] presented the weak gravity conjecture (WGC). The WGC is stated as “there is no monopole heavier than any black hole”. It is stated in Ref. [115] that there is a new hidden cut-off scale Λ below the Planck mass M_{P} .

Let us proceed to discuss wormholes. Irrespective of the validity of the WGC, the wormhole consideration does not allow exact global symmetries. Any global symmetry we have considered in Chapter 6 must be approximate. In Fig. 6.23, a 4-manifold is shown. The observable Universe O we live in is shown on the LHS, and the shadow world S is shown on the RHS. A wormhole connects the observable

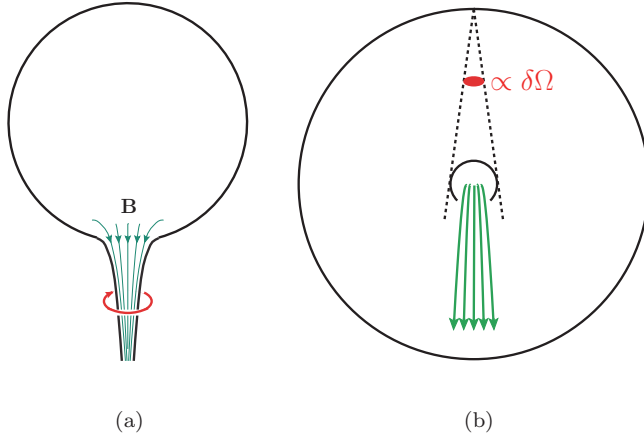


Fig. 6.22. A black hole throwing out magnetic field B .

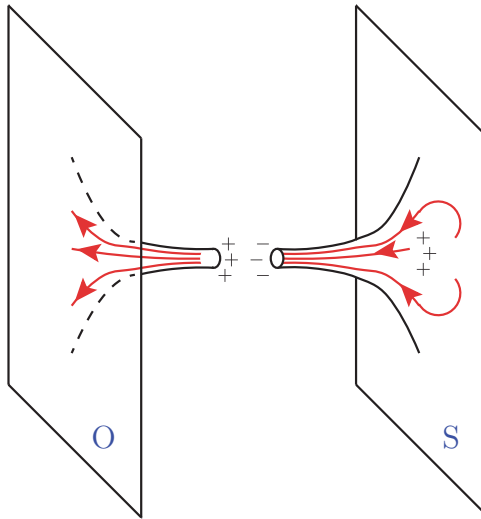


Fig. 6.23. A wormhole connecting the visible Universe and a shadow world.

world O to the shadow world S. Let us consider a $U(1)$ gauge symmetry. For a non-Abelian group, one may consider just a $U(1)$ subgroup. If a $U(1)$ gauge charge, e.g., the electromagnetic charge e , is flown to the shadow world, it drags the flux lines. The effect of this metric change appears to the observer O as an effective interaction. The effective interaction in the observable Universe is obtained by cutting off the shadow world, i.e., by chopping off the neck of the wormhole. Note then that the same amount of the flown-out charges are recovered to the observer O as depicted in Fig. 6.23. Then, the observer O considers that the gauge symmetry $U(1)$ is not broken by the wormhole.

6.6.2. *Discrete symmetries: top-down*

So, possible discrete symmetries not affected by gravity were suggested to be subgroups of gauge symmetries, for which “discrete gauge symmetry” was invented [116]. Some useful discrete symmetries used for stability of particles are baryon number, lepton number, and R parity in supersymmetry.

For global symmetries, topology change by black holes and wormholes can take out charges from our observable Universe O , which was used to limit the application of the PQ symmetry toward the solution of the strong CP problem [117]. The flux line argument discussed above for gauge symmetries that does not apply to global symmetries guarantees that topology change does not break gauge symmetries because the observer O confirms that gauge charges are not lost through a wormhole as depicted in Fig. 6.23. Note, however, that the renormalizability of gauge theory interactions is not used in this argument of flux lines. The flux lines are based on the equation of motion which is a classical concept. Thus, the underlying renormalizable gauge theory and hence the resulting “discrete gauge symmetry” [116] are an over-requirement.

However, if the flown-out charges are global charges, then they do not drag flux lines and the observer O considers that he lost the global charges. The PQ global symmetry is a handy example illustrating the wormhole and black hole breaking of global symmetries. This point was stressed in Ref. [117] with f_a in the axion window, $10^9 \text{ GeV} \leq f_a \leq 10^{11} \text{ GeV}$. This is because the PQ global symmetry has the color anomaly.

6.6.3. *Discrete charges and discrete flux*

For a gauge (local) symmetry with the current conservation, the Gauss theorem due to the long range force defines the corresponding gauge charge inside a sufficiently large sphere. The information on the flux of gauge fields at the surface enables one to figure out the charges inside the sphere.

For a global symmetry with the current conservation, there is no corresponding gauge fields at the surface and the global charge inside the sphere cannot be calculated by the information at the surface.

Figure 6.24 is shown to figure out how the discrete charge inside a closed surface is estimated. The yellow vacuum does not carry discrete charge. The red vacuum carries some discrete charge. The black bullets are particles carrying discrete charges. The walls between the yellow and red vacua are visualized by the limegreen color. If only particles are present in the yellow vacuum, there will be no such wall.

In Section 6.6.2, the discrete gauge symmetry has been discussed in the top-down approach. It was designed to be a subgroup of a gauge symmetry. There the flux line argument was used for gauge symmetries. In this section, we argue in the bottom-up approach, considering only the discrete charges in terms of low energy fields and their discrete charges. For discrete symmetries, note that they are

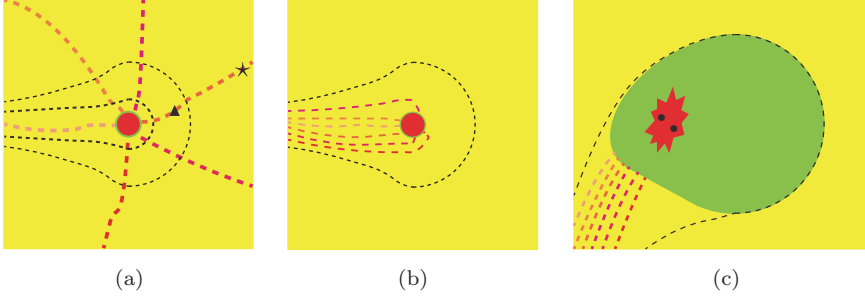


Fig. 6.24. (a) A $\mathbf{Z}_N$ -walled ball seen in the $\phi = 0$ vacuum. The tail of the “tadpole” can have $n = 0, 1, \dots, N - 1$ dashed lines. N dashed line is equivalent to no tail, i.e., no $\mathbf{Z}_N$ charge. (b) Another view of (a) by the discrete flux, and (c) an expanded view of (b) with the dashed boundary touching the wall. In (a), the discrete charges inside two dashed surfaces are the same.

defined together with walls in the Universe. Note that the vacua are defined by the VEVs of Higgs fields. In Fig. 6.24(a), we enclose the discrete charges by two dashed surfaces: the thick and thin ones. The discrete charges inside the thin and thick surfaces are exactly the same. If we assign one discrete charge to one dashed red line, the Higgs vacuum value at the star at the dashed line is the same as that at the triangle because they are at the same $q = 0$ (i.e., Higgs field = constant) vacuum. For $\mathbf{Z}_N$ with $q = 1, 2, \dots, N - 1$, a kind of strings are drawn in Fig. 6.24(a) where $q = 6$. Thus, calculating the discrete charge in Fig. 6.24(a) is the same as that calculated in Fig. 6.24(b). Also, it is like calculating the discrete charge in Fig. 6.24(c) where we made it clear by moving the dashed surface touching the wall at the RHS of Fig. 6.24(c). So, when discrete charges move, we can consider them dragging dashed lines corresponding to some units of discrete charges. This conclusion will not be changed in case there are some particles in the $q = 0$ vacuum without the wall. The total discrete charge inside the dashed wall of Fig. 6.24 is given by

$$Q_{\text{total}} = \sum_i Q_i + \frac{1}{2i} \int_{(\text{red ball})} d^3x (\phi^* \partial_t \phi - \phi \partial_t \phi^*), \quad (6.193)$$

where Q_i is the discrete charge of particle i inside the dashed surface.

Now, let us consider $\mathbf{Z}_2$ [118]. In Fig. 6.25, the $q = 0$ and 1 vacua are shown together with some particles (black bullets of Fig. 6.25). Let us consider Fig. 6.25(a). In case of the $q = 1$ vacuum, Fig. 6.25(b), we can apply a discrete transformation $e^{i\pi q}$ and use the argument presented for Fig. 6.25(a). So, consider Fig. 6.25(a) without loss of generality. Through wormholes, discrete charges can flow out from our Universe O. An infinite-tail $\mathbf{Z}_2$ “tadpole” is symbolized in Fig. 6.26(a), where $Q_{\text{total}} = 1$. The “tadpole” tail extends to horizon or ends at the “tadpole” head. Discrete charge flow can be visualized as a “tadpole” passing through the wormhole as shown in Fig. 6.26(b). If one tries to separate the shadow world S from O by cutting the wormhole through the gray plane in Fig. 6.26(b), it cuts the “tadpole”,

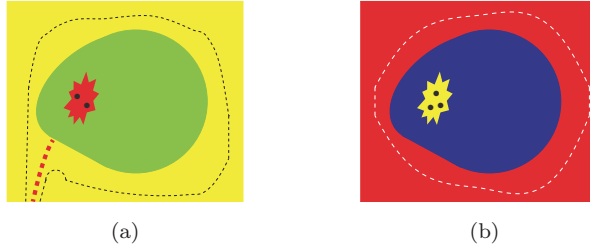


Fig. 6.25. Domains, walls, and string with $\mathbf{Z}_2$ symmetry. (a) A walled ball seen in the $q = 0$ (yellow) vacuum with $Q_{\text{total}} = 1$. Inside the wall, the opposite $q = 1$ (red) vacuum is seen through a crack in the wall. This view of the wall is colored limegreen. (b) A walled ball seen in the $q = 1$ (red) vacuum with $Q_{\text{total}} = 0$. This view of the wall is colored blue. Black dots in the balls are particles.

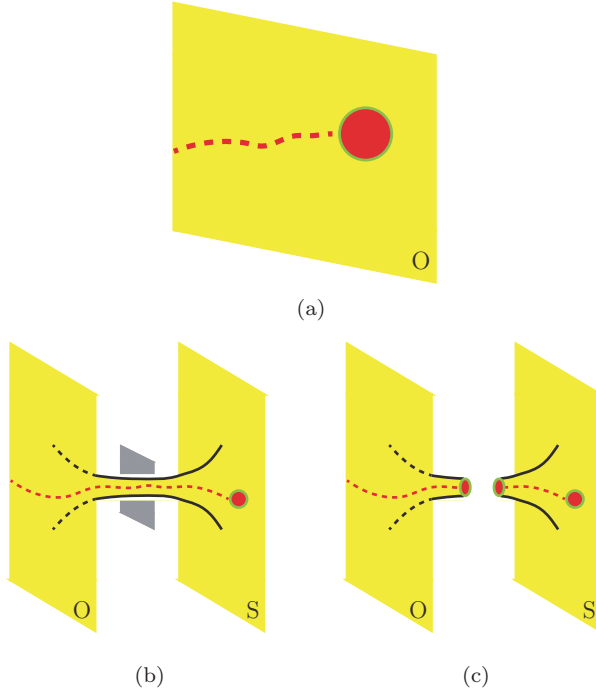


Fig. 6.26. (a) A walled ball seen in the $\phi = 0$ vacuum. The tail of a tadpole-like configuration extends to the horizon. (b) A tadpole passing through a wormhole. (c) The wormhole cut in the gray plane in (b). The observer O recovers the discrete charge.

and the cut dashed lines at the cut plane are attached to a walled ball at each surface as shown in Fig. 6.25(c). Recovering the wormhole throat, the observer O confirms that no discrete charge is lost. Thus, to the observer O, gravitational effects do not break the discrete symmetry $\mathbf{Z}_2$ in consideration. For $\mathbf{Z}_N$, the argument must be similar.

6.6.4. Gravity effects to discrete symmetries

All discrete symmetries can be embedded as some subgroups of continuous groups, gauge, or global. We argued in the bottom-up approach of Section 6.6.3 that a $\mathbf{Z}_N$ discrete symmetry is not spoiled by gravity. If a discrete symmetry is embedded to a gauge group, these discrete symmetries are called *discrete gauge symmetries* [116]. For the discrete gauge symmetry, different vacua of Higgs fields have degenerate potential energy. To have walls between different vacua, the discrete symmetry must be broken at low energy. Consider an example of a U(1) gauge symmetry broken down to $\mathbf{Z}_2$ at the scale v_{high} by the VEV of Higgs field carrying U(1) gauge charge 2. Then, consider another Higgs field carrying U(1) gauge charge 1, developing a VEV at v_{low} . Then, the energy density of the domain wall is given by $\propto v_{\text{high}}^3 v_{\text{low}}$. We can generalize this gauge symmetry to include the Lorentz symmetry. This is because by extending the Lorentz symmetry to a local one, we can consider gravity-field flux lines in Fig. 6.23, instead of gauge-field flux lines, and the recovered charge is the energy-momentum.

Now, we can define *discrete global symmetries*. Since our mother continuous symmetries are hypothetical, the distinction between discrete gauge and global symmetries is only by checking whether the mother continuous symmetry has gauge anomalies or not. If there is no gauge anomaly of the mother continuous symmetry, then the son discrete symmetry must be discrete gauge symmetry discussed above. If the mother continuous symmetry has some gauge anomalies, then the son discrete symmetry cannot be discrete gauge symmetry, and we consider it as discrete global symmetry. For the walls to be present between discrete vacua, there must be a symmetry breaking barrier between the walls. It is provided by the breaking terms of the mother continuous symmetry as illustrated in Fig. 6.13. For the energy barrier to be present in discrete gauge symmetries, the $\mathbf{Z}_N$ symmetry must be broken at a lower energy scale as discussed above.

Looking at just a low energy effective theory, there is no way to know how the high energy fundamental theory produced the low energy discrete symmetries. But, there is a big difference between discrete gauge and discrete global symmetries. For discrete global symmetries, we need not break the discrete symmetry further if gauge anomalies already break the global symmetry. In this case, the wall between different Higgs vacua can be present with the exact discrete global symmetries (except the anomaly). If there is no gauge anomaly, the wall energy can be provided some term in the potential breaking of the global symmetry. On the other hand, discrete gauge symmetries do not provide the wall energy.

It is known that discrete symmetries $\mathbf{Z}_{N_{\text{DW}}}$ present in axion models are exact (except the QCD anomaly) as discussed above because the mother continuous symmetry is the PQ global symmetry. These exact discrete symmetries broken spontaneously in the cosmos lead to serious domain-wall energy crisis if N_{DW} is not one as discussed in Section 5.3. However, if the axion vacua of the PQ global symmetry are connected by another independent direction, we can identify different PQ vacua

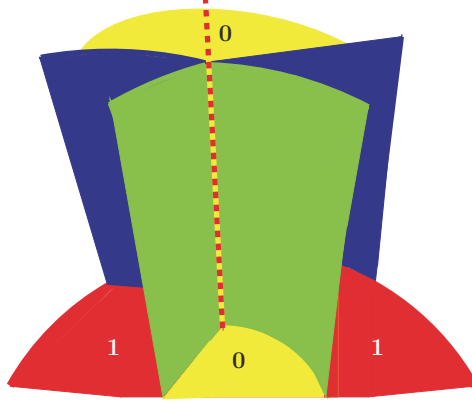


Fig. 6.27. Generation of a two-dimensional delta function from the $\mathbf{Z}_2$ boundaries of vacua.

and we obtain $N_{\text{DW}} = 1$. For this identification, the center of gauge groups and the Goldstone boson direction have already been discussed in relation to Fig. 5.8.

Let us illustrate how such a string is set up in the spontaneously broken $\mathbf{Z}_2$ vacua [118]. Let us consider a dash surface of Fig. 6.25(a) in the case of $\mathbf{Z}_2$. Our objective is to obtain a two-dimensional delta function into the (r, θ_0, ϕ_0) direction in the spherical-polar coordinate system. Consider the $\mathbf{Z}_2$ symmetric action,

$$\frac{1}{M} \partial^\mu \partial^\nu \Psi^* \partial_\mu \partial_\nu \Psi, \quad (6.194)$$

where the Lorentz symmetry is broken in the vacuum we consider in Fig. 6.25(a). We can consider the following two-index current and one-index charge:

$$\propto i (\Psi^* [Q_\Psi \partial^\mu \partial^i \Psi] - [Q_\Psi \partial^\mu \partial^i \Psi]^* \Psi) \rightarrow Q^i = \frac{1}{M} \int d^3 x \Psi^* \partial^0 \partial^i \Psi, \quad (6.195)$$

where M is a scale parameter. The current conservation implies

$$\partial_\mu j^{\mu i} = 0 \rightarrow Q^i = \frac{1}{M} \int_V d^3 x \frac{\partial}{\partial x^j} j^{ji} = \frac{1}{M} \int_{\Sigma_r} d^2 \sigma_r j^{ri}, \quad (6.196)$$

where Σ_r is the surface orthogonal to the radial direction. So for discrete values of $q = 0$ and 1, we have for a string in the (θ_0, φ_0) direction,

$$j^{\theta \varphi} = \frac{1}{r^2} \delta(\cos \theta - \cos \theta_0) \delta(\varphi - \varphi_0), \quad (6.197)$$

since derivative of a step function gives a delta function. It is shown in Fig. 6.27.

6.6.5. With extra dimensions

In case the observable Universe is connected by a wormhole to a shadow world with the extra dimensions, consider cutting off the wormhole. As commented before, we note especially that the eigenvalues of the higher dimensional Lorentz generators are

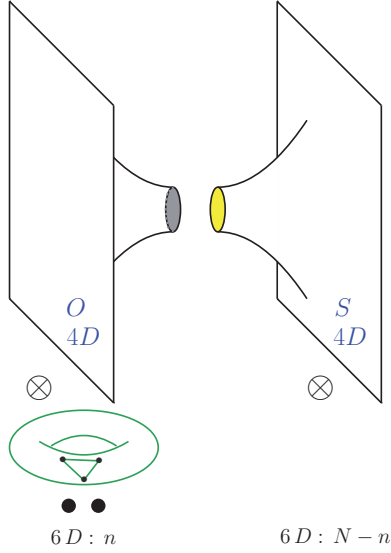


Fig. 6.28. Compactification of six internal dimensions with $\mathbf{Z}_N$ discrete symmetry in 4D.

not lost by this action. In the heterotic string compactification, they are 4D Lorentz generators and discrete symmetries arising from the internal six dimensions.

Compactification of six internal dimensions can also lead to discrete symmetries. This belongs to 10D Lorentz group. In Fig. 6.28, we depict the splitting of 10D to (4D Minkowski space) $\otimes$ (six compact dimensions) for the case of a $\mathbf{Z}_N$ discrete symmetry. In Fig. 6.12, we showed $\mathbf{Z}_2$ vacua. If we cut at the top of a hill, the two different sides with different eigenvalues of $\mathbf{Z}_N$ are separated as we showed for the case of $\mathbf{Z}_2$ in Fig. 6.26.

In 10D heterotic string theory, the mother continuous symmetry must be $E_8 \times E_8'$ times 10D Lorentz symmetry. The part of Lorentz symmetry belonging to 4D Minkowski space is used for SUSY WIMPs. The R-parity is given by $R_P = (-1)^{3B-L+2S}$ [119]. The spin S is the charge belonging to the 4D Lorentz transformation. Baryon number B and lepton number L are generators of global symmetries in the standard model and hence R-parity R_P is approximate in the sense of Fig. 6.13. Usually, R_P in 4D is considered as a subgroup of a global $U(1)_R$. But from the compactification, the mother continuous symmetries are gauged. So, the approximate level, determining the domain wall energy density, is determined by the Higgs vacua with a VEV at high energy v_{high} and a VEV at low energy v_{low} . The lightest R-parity odd particle called the LSP is the main focus of SUSY WIMP in Chapter 7.

Exercise

1. Show that Eq. (6.5) is the solution of Eq. (6.4).

2. Find the form of the solution (6.19) with a trick of using integral transformation,

$$\tilde{g}(s) = 2 \int_0^\infty dt \frac{t^{\frac{1}{\alpha}+1}}{s^{\frac{1}{\alpha}+2}} e^{-(t/s)^2} g(t) \quad (6.198)$$

with $g(t) = t^{2k}$.

3. By redefining a_{IJ} and b_{IJ} , show that Eq. (6.68) is equivalent to the following:

$$\begin{aligned} V_W = \frac{1}{2} \sum_I m_I^2 \phi_I^\dagger \phi_I + \frac{1}{4} \sum_{IJ} [a_{IJ} \phi_I^\dagger \phi_I \phi_J^\dagger \phi_J + b_{IJ} \phi_I^\dagger \tau^i \phi_I \phi_J^\dagger \tau^i \phi_J \\ + c_{IJ} \phi_I^\dagger \phi_J \phi_I^\dagger \phi_J] + \text{h.c.}, \end{aligned} \quad (6.199)$$

where τ^i are the $\text{SU}(2)_L$ generators on doublets.

4. Show that Eq. (6.99) holds when the $\text{SU}(2)$ isospin is not broken.
 5. Obtain the axion lifetime given in Eq. (6.140).
 6. Obtain the entries of Table I of Ref. [37]. Refer to Example 7.1 of Chapter 7.

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Chapter 7

WIMPs and E-WIMPs

It is the general rule that the originator of a new idea is not the most suitable person to develop it, because his fears of something going wrong are really too strong — P. A. M. Dirac

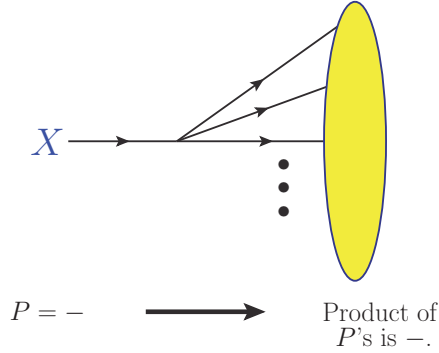
Basics on the WIMP (weakly interacting massive particle) have been already discussed in detail at several places in this book, as presented in Chapter 2, and Sections 4.2, 4.5, 5.3, and 6.6. In fact, the main theme in the cold dark matter (CDM) discussion in this book, except the bosonic collective motion discussed in Chapter 6, is based on the WIMP idea. Therefore, here we will pay attention to the particle physics aspects on the particles useful for WIMPs and their possible interactions. This chapter is a brief summary of theories on WIMPs and E-WIMPs.

The underlying symmetries of WIMPs are discrete and global symmetries. The R -parity in supersymmetry (SUSY) is a good discrete symmetry example, and a dark number (a mimic of baryon number) in the asymmetric dark matter (ADM) scenario is a global symmetry example. WIMPs are discussed in this chapter except the ADM which will be discussed in the next chapter.

Solving the Boltzmann equation for the DM density n_{DM} , the equilibrium number density in the nonrelativistic regime is given by

$$n_{\text{DM}} = g_* \left(\frac{m_{\text{DM}} T}{2\pi} \right)^{3/2} e^{-m_{\text{DM}}/T}, \quad (7.1)$$

where g_* is the number of spin degrees of freedom. Here, the temperature T is identical to that of a thermal plasma, i.e., an entropy sector where $T \propto 1/a$ (from comoving entropy density conservation), as long as the WIMPs are in kinetic equilibrium with the plasma.

Fig. 7.1. Decay of a P odd particle.

7.1. Discrete symmetries

The presence of weakly interacting massive particles (WIMPs) in the Universe is an inevitable consequence if there exist some exact discrete symmetries. Discrete symmetries in the cosmos were briefly reviewed in Section 6.6. The most widely used discrete symmetries for WIMPs are $\mathbf{Z}_2$ and parity. In two dimensions, parity operation is identified with Z_2 . The $\mathbf{Z}_2$ and parity operations in two dimensions are

$$Z_2 : re^{i\theta} \rightarrow re^{i(\theta+\pi)}, \quad (7.2)$$

$$P : \begin{cases} x \rightarrow -x, \\ y \rightarrow -y. \end{cases} \quad (7.3)$$

Since $x = r \cos \theta$ and $y = r \sin \theta$, they are identical. For $\mathbf{Z}_N$ with $N \geq 3$, there is no such relation. But for mirror reflection instead of parity, one can find a relation.

For a larger discrete symmetry, there are larger representations of the discrete group in which case multiple degenerate WIMPs are expected. Therefore, there is no need for a bigger discrete group toward WIMPs at present. So, we focus on $\mathbf{Z}_2$ and parity in this chapter.

7.1.1. Parity eigenstates

Eigenvalues of P are customarily represented as $+$ (even) and $-$ (odd), which correspond to $\mathbf{Z}_2$ eigenvalues of $2n, 2n+1$ ($n = \text{integer}$), respectively. An interaction term is allowed if its P eigenvalue is even and forbidden if it is odd. The standard model (SM) particles are denoted as parity even states, and hence the interactions of the SM are all allowed without extra constraints.

Suppose that a $P = \text{odd}$ particle decays as shown in Fig. 7.1. Since the total eigenvalue of the final state particles is the product of all final state P eigenvalues, the least possible number of P odd final states is one. Therefore, the lightest P odd

particle (LPOP) cannot decay to any other particle(s). This LPOP is a candidate for the dark matter (DM) WIMP.

In the literature [1], non-Abelian discrete symmetries have been considered, mainly for the lepton mass matrix texture. However, these may not be so useful for the case of the WIMP because “non-Abelian” discrete symmetry group by definition includes many nonsinglet representations while in the WIMP context we discuss only one absolutely stable particle. Therefore, in this case it is proper to consider a $\mathbf{Z}_2$ subgroup of such a non-Abelian discrete group. In this sense, the DM stability is not due to the non-Abelian nature but to the group $\mathbf{Z}_2$ [2].

The first cosmological study of a heavy stable particle interacting weakly with the visible-sector particles was performed by Hut [3] and Lee and Weinberg [4] based on $2 \rightarrow 2$ interaction as discussed in Chapter 2. This was followed by Goldberg [5] for the case of photino in SUSY context and has been reviewed extensively in [6]. In Fig. 1.4, we listed several WIMP candidates in the cross-section vs. mass plot, where σ_{int} is the typical strength of the $2 \rightarrow 2$ interactions with ordinary matter. There, the red, pink, and blue colors represent hot, warm, and cold DMs, respectively. For the case of SUSY WIMPs, a $\mathbf{Z}_2$ symmetry was needed, which is usually taken to be R -parity in which case the LPOP is the lightest SUSY particle (LSP) in most models. Other unbroken discrete symmetries are also possible for an absolutely stable particle in SUSY models [7]. Recently, strongly interacting massive particles (SIMP) in the MeV scale have been suggested for DM possibility based on the dominant $3 \rightarrow 2$ interaction compared to $2 \rightarrow 2$ interaction [8]. If a $4 \rightarrow 2$ interaction dominates, the SIMP mass scale can be as low as keV.

7.1.2. $\mathbf{Z}_2$ as a discrete subgroup of $U(1)$

The LPOP can be replaced with the lightest $\mathbf{Z}_2$ odd particle (L $\mathbf{Z}_2$ OP). One can consider a $\mathbf{Z}_2$ subgroup of a $U(1)$ gauge symmetry [9]. But, we can consider a global $U(1)$ also as reviewed in Section 6.6. Let the generator of $U(1)$ be Q , and under a gauge transformation by α the scalar field ϕ transforms as $\phi \rightarrow e^{i\alpha Q}\phi$. Now Q is normalized such that the smallest nonzero value of the Q eigenvalues of the fields in the full theory is 1. So, for a nonzero $Q(\phi)$, $|Q(\phi)|$ is ≥ 1 . Suppose that $Q(\phi) = N$ with the integer N greater than 1. Then, under a full rotation of the gauge parameter α from 0 to 2π , the phase of ϕ rotates by $2\pi N$. For ϕ , $\alpha = [0, 2\pi N)$ is the physical region. Namely, for ϕ , $\alpha = 2\pi N$ is identified with 0. However, for some other fields, transformation $\alpha = [0, 2\pi N)$ might have repeated the fields more than once. It defines the domain wall (DW) number of the theory: $N = N_{\text{DW}}$. Thus, if ϕ develops a VEV, $\langle \phi \rangle = v$, the $U(1)$ gauge symmetry is broken but the integer shift $\alpha = n$ ($0 \leq n < N$) defines multiple vacua. In this case, the gauge/global symmetry is broken down to the discrete symmetry $\mathbf{Z}_N$. To illustrate this, consider an interaction

$$\Psi_1 \Psi_2 \Phi, \quad (7.4)$$

where Q eigenvalues of Ψ_1, Ψ_2 , and Φ are $n_1, -N - n_1$, and N , respectively. Certainly, the interaction term respects the $U(1)$ gauge symmetry. By the VEV of ϕ , the $U(1)$ gauge symmetry is broken to $\mathbf{Z}_N$. The $\mathbf{Z}_N$ eigenvalue of Ψ_1 is $n_1 \bmod N$, the $\mathbf{Z}_N$ eigenvalue of Ψ_2 is $-N - n_1 \bmod N$, and the $\mathbf{Z}_N$ eigenvalue of Φ is $N \bmod N$. Thus, the $\mathbf{Z}_N$ value of the interaction (7.4) is $n_1 - N - n_1 + N = 0$. Even if the gauge/global $U(1)$ is spontaneously broken, the $\mathbf{Z}_N$ symmetry is a good symmetry of the interaction. But, for the DW energy density to be present, the $\mathbf{Z}_N$ symmetry from a gauge $U(1)$ must be broken explicitly. For the DW energy, the $\mathbf{Z}_N$ symmetry from a global $U(1)$ might have been broken by anomaly as discussed in Section 6.6 and if it were not broken by anomaly, then an explicit breaking term is also needed.

Thus, there can be numerous models for WIMPs without concern for gravity. The most widely discussed WIMP is the LSP with R -parity defines as [10],

$$R_P = (-1)^{3B-L+2S}, \quad (7.5)$$

which is the standard candle in the SUSY WIMP detection.

7.2. Weakly interacting massive particles (WIMPs)

7.2.1. Interaction mediators

An approximate solution of the Boltzmann equation provides the present day thermal WIMP relic density, Eq. (7.1), expressed in terms of cosmologically relevant parameters as [11],

$$\Omega_X h^2 \simeq \frac{s_0}{\rho_c/h^2} \left(\frac{45}{\pi^2 g_*} \right)^{1/2} \frac{1}{x_f M_P} \frac{1}{\langle \sigma_{\text{ann}} v \rangle}, \quad (7.6)$$

where s_0 denotes the present day entropy density of the Universe, g_* the number of relativistic degrees of freedom at freeze-out and

$$x_f \equiv \frac{T_{\text{fr}}}{m_X}, \quad (7.7)$$

which is the freeze-out temperature scaled to m_X . Numerically, x_f is $\approx 1/25$. Plugging the known values for s_0 and ρ_c , and setting $\Omega_X h^2$ to its measured value $\simeq 0.12$, one finds

$$\frac{\Omega_X h^2}{0.12} \simeq \frac{1}{\langle \frac{\sigma_{\text{ann}}}{10^{-36} \text{ cm}^2} \frac{v/c}{0.1} \rangle}. \quad (7.8)$$

Thus, an annihilation cross-section of weak strength of order 10^{-36} cm^2 and typical WIMP velocities at freeze-out give the correct present day CDM density. Thus, masses of the interaction mediators are expected to be of order 100 GeV.

The TeV scale SUSY introduces superpartners of the SM particles around the TeV scale, which can work as interaction mediators. This has been the most

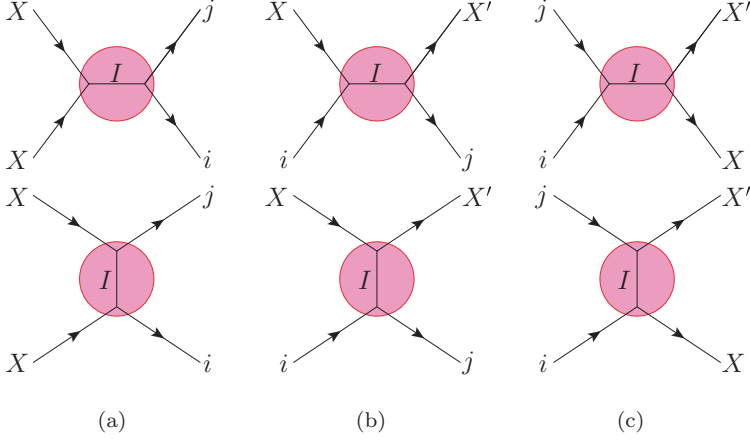


Fig. 7.2. The WIMP interactions, (a) in their annihilation, (b) in the detection experiments, and (c) in the production at high energy colliders. i and j are the SM particles, and I is the force mediator.

attractive cosmological reason for the TeV scale SUSY particles. With one hypothesis of SUSY at TeV scale, one can understand both the gauge hierarchy and the CDM WIMP density. Note, however, that the ATLAS and CMS experiments at the Large Hadron Collider (LHC) [13] excluded gluino mass smaller than 1.8 TeV from the motivated decay mode

$$p + p \rightarrow \tilde{g} + \tilde{g}, \quad \tilde{g} \rightarrow t + \bar{t} + \chi_1^0. \quad (7.9)$$

This problem has led to considering numerous other CDM particles. For other WIMP suggestions, however, the relation between the theory motivation and CDM density is not always automatic. Therefore, we will pay much attention on the LSP in this chapter, at least for a prototype example.

In Fig. 7.2, we present three types of Feynman diagrams where WIMPs participate in the scattering processes. Figure 7.2(a) is the WIMP annihilation diagram, for the s - and t -channels, which determine the WIMP density at the freeze-out temperature, given in Eq. (7.8). X is a WIMP, i, j are the SM particles, and I is the force mediator. Figure 7.2(b) is the WIMP detection diagram used in the direct WIMP search experiments. Figure 7.2(c) is the WIMP production diagram at high energy accelerators as in the LHC. In all these diagrams, there appear the intermediate particle I , the force mediator.

Figure 7.2(b) is also the diagram establishing the kinetic equilibrium temperature T given in Eq. (7.1). The kinetic interaction can even change [12] the relic abundance in nonthermal production scenarios [11].

The mass parameter M_X appearing in Eq. (7.7) is in fact a combination of the mass of X and the mass of force mediators. In many cases, these are taken as the same. But, in detail a combination must appear. For example, for a heavy $SU(2)_L$ doublet neutrino case N , the force mediator is $W^\pm$ and the X particle mass is the

Table 7.1. The MSSM particles.

Species		Superpartners	
u -type Higgs doublet	H_u	$\tilde{H}_u$	u -type higgsino doublet
d -type Higgs doublet	H_d	$\tilde{H}_d$	d -type higgsino doublet
photon	γ	$\tilde{\gamma}$	photino
neutral weak boson	Z^0	$\tilde{Z}$	zino
charged weak boson	$W^\pm$	$\tilde{W}^\pm$	wino
gluons	g	$\tilde{g}$	gluinos
electron-neutrino, ...	ν_e, ν_μ, ν_τ	$\tilde{\nu}_e, \tilde{\nu}_\mu, \tilde{\nu}_\tau$	s-neutrinos
electron, muon, tau	e, μ, τ	$\tilde{e}, \tilde{\mu}, \tilde{\tau}$	selectron, s- μ , s- τ
$Q_{\text{em}} = \frac{+2}{3}$ quarks	u, c, t	$\tilde{u}, \tilde{c}, \tilde{t}$	scalar u -quark, squarks
$Q_{\text{em}} = \frac{-1}{3}$ quarks	d, s, b	$\tilde{d}, \tilde{s}, \tilde{b}$	scalar d -quark, squarks
graviton	$g_{\mu\nu}$	$\tilde{G}$	gravitino

In the last row, we included gravitino.

heavy neutrino mass m_N . Scatterings and decay of N depend on two parameters M_W and m_N [4]. For the LSP, the force mediator can be probably relatively light SUSY particles. Because there are so many SUSY particles, it is difficult to pinpoint the mass parameter in terms of masses of interaction mediators, which is the reason that the LSP searches are summarized as figures for certain assumptions on masses.

7.2.2. *SUSY WIMPs*

The R -parity odd WIMP, in particular in the MSSM, has been studied in Section 4.9.1. In Table 7.1, we list the SM particles of Fig. 1.1 and their SUSY partners, which constitute the MSSM model.

The LSP was considered as photino, bino, or stau, etc. In most cases, the LSP usually denoted as $\chi = X$ is a combination of neutral wino $\tilde{W}^0$, bino $\tilde{B}^0$, neutral up-type-higgsino $\tilde{H}_u^0$, and neutral down-type-higgsino $\tilde{H}_d^0$. These neutralinos interact with MSSM intermediate states and their superpartners. For any Feynman diagram allowed in the SM, one can replace a continuous line by the superpartner of the corresponding SM particle. In Fig. 7.3, starting from the t -channel $e^+e^- \rightarrow 2\gamma$ diagram, we draw an SUSY diagram by replacing one continuous line by the superpartner of the SM particle, i.e., $\tilde{e}^-$. Since there are so many possible intermediate state particles I for diagrams of Fig. 7.2 in the MSSM, an easy analysis of the cross-section calculation in the MSSM is not possible. In the analysis, one must satisfy other phenomenological constraints on the MSSM parameters.

The unknown parameters in the MSSM are masses of photino, zino, wino, gluino, Higgsino, sleptons, and squarks. A total number of these parameters are about 100. To simplify the analysis, usually a simplified version, the so-called constrained MSSM (CMSSM) (or mSUGRA) in supergravity is used where the gaugino mass unification and the universal scalar masses ($= m_{3/2}$) at M_{GUT} are adopted. In

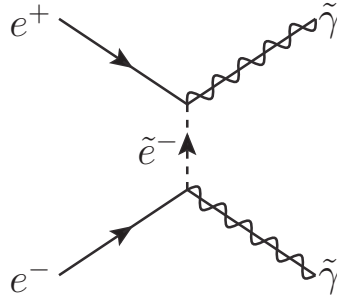
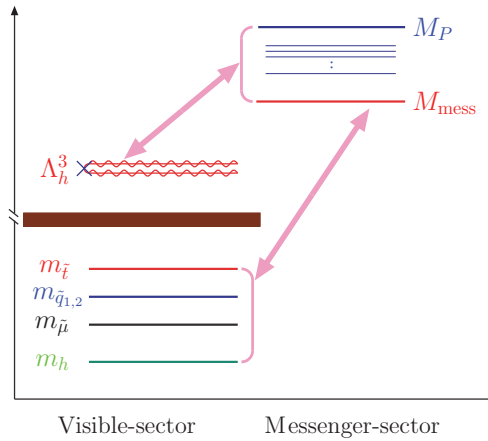


Fig. 7.3. A photino production diagram.

Fig. 7.4. The messenger scale for transmitting SUSY breaking Λ^3 down to the electroweak scale.

this case, there are five parameters: the universal gaugino mass $m_{1/2}$, the universal soft mass m_0 for squark, sleptons and Higgs scalars, the A -term mostly dominated by the t -quark mass, $\tan\beta = v_u/v_d$, and the sign of μ term [14]. The TeV scale gluino, wino, neutralino, and sfermion masses are obtained by running them from M_{GUT} down to the electroweak scale. Here, it is usually assumed that the SUSY breaking scale at Λ_h transmitted down by some nonrenormalizable interactions. The mass scale appearing in the denominator of the effective interaction is called the “messenger scale”. The mass spectra in the CMSSM are schematically shown in Fig. 7.4. The Planck mass M_P and the GUT scale M_{GUT} are two popular messenger scales.

7.2.3. Non-SUSY WIMPs: With SM gauge group in 4D

A particle X with mass m_X is absolutely stable if there are no particles lighter than the sum of masses of those particles whose total quantum number is equal to

that of X : i.e., $m_X < \sum m_i$. Both proton and electron are prototypical examples of stable particles whose stability arises from a symmetry principle: in the former case from the baryon number conservation while in the latter case from the electric charge conservation. These are the charges corresponding to the global symmetry $U(1)_B$ and the gauge symmetry $U(1)_{\text{em}}$. Proton is the lightest particle carrying the baryon number B . Similarly, the lepton number L is used for conserving the lepton number. Below the proton mass, there is no lighter color-singlet particle carrying baryon number and proton cannot decay. Thus, proton is absolutely stable if the B conservation is exact. However, in theories where B and L are broken — i.e., in GUTs — the proton can decay to lighter particles such as by the process $p \rightarrow e^+ \pi^0$. If one uses a discrete symmetry, a similar argument can be used: if there is no combination of lighter particles with the same discrete quantum number of X with mass below m_X , then X is absolutely stable if the discrete symmetry is exact. If the discrete symmetry is broken, then X is not absolutely stable.

We list some DM candidates which can be interpreted as WIMPs, starting from the simplest SM case and progressing into more complex cases.

In this chapter, two Higgs doublets of the SM are denoted as

$$\begin{aligned} H_d &= \begin{pmatrix} H_d^0 \\ H_d^- \end{pmatrix}, & H_u &= \begin{pmatrix} H_u^+ \\ H_u^0 \end{pmatrix}, \\ Y &= -\frac{1}{2}, & Y &= +\frac{1}{2}, \end{aligned} \tag{7.10}$$

which are assumed to carry no global quantum numbers.

Sterile neutrino

All SM singlet fermions with parity even quantum number can be called sterile neutrinos. The masses of these singlets can range from well below the electroweak scale to the Planck scale. Here, let us concentrate on keV scale singlet neutrinos.¹ They arise in the following set up.

Consider the electron family and a sterile neutrino,

$$\ell_e = \begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \quad e_L^c, \quad N_L, \tag{7.11}$$

where we used the left-handed chirality. Considering only kinetic energy terms and the Yukawa coupling $\ell_e e^c H_d$, one finds that there are two global symmetries, the electron number and the N number, for which ν_e and e carry $L_e = 1$ and $L_N = 0$, and N carries $L_e = 0$ and $L_N = 1$. Thus, the massless sterile neutrino N is absolutely stable. Next, introducing the mass term of N by $\frac{m_N}{2} N^T C^{-1} N$, the N

¹Possible cases are reviewed in Ref. [15].

number is broken. At this stage, the electron number is conserved. Finally, let us introduce a renormalizable coupling

$$f_N (\nu_e, e)_L^T C^{-1} (i\sigma_2) N_L \begin{pmatrix} H_u^+ \\ H_u^0 \end{pmatrix} + \text{h.c.}, \quad (7.12)$$

where $i\sigma_2$ acts in the $SU(2)_L$ space. This interaction identifies $L_N = -L_e$. But, the L_N is broken by the mass term and so is L_e . The degree of validity of using L_e is due to the magnitude of red terms in Fig. 4.5. The leading term in the red is the dimension 5 operator

$$\frac{f_N^2}{m_N} (\nu_e, e)_L H_u (\nu_e, e)_L H_u \quad (7.13)$$

which gives the electron neutrino mass of order v_u^2/m_N . It is the seesaw mechanism [16].

Most sterile neutrino scenarios forbid the Majorana mass term of N' by the assumption. Then, the Dirac mass term $\bar{\ell}_e N'_L \langle H_d \rangle$ is the neutrino mass term and relates $L_e = L_{N'}$. In this case, the lepton number L_e is not broken. In addition to three lepton families, let us introduce two SM singlet neutrinos

$$N'_L, \quad N'_L{}^c, \quad (7.14)$$

and introduce a Dirac neutrino mass $m_{N'} \bar{N}'_R N'_L{}^c$ but no Majorana mass is introduced. There is an additional conserved number $L_{N'}$. At this stage, there are two conserved numbers, L_e and $L_{N'}$. Now, allowing the coupling $f_{eN'} \bar{\ell}_e N'_L H_d$, there remains only one conserved number, $L_e = L_{N'}$.

Let us start the sterile neutrino discussion from this set up. N' is called “sterile” neutrino because it, being neutrino, does not carry any SM gauge quantum number. If N' is heavier than the three neutrinos of the SM, it will decay to a neutrino plus photon, via the one-loop diagram with the H_u^- exchange in the loop. Superheavy neutral leptons N' s, presumably three of them as in the SM, are assumed to have Majorana masses for the seesaw masses of the SM neutrinos. Three lepton families mix. Disregarding the Majorana masses of N' s for a moment, we have one conserved lepton quantum number, i.e., $L_{N'} = L_e = L_\mu = L_\tau$. In the effective theory of the light particles of the SM, the lepton number violation is tiny, and the $L_{N'}$ number conservation can be effectively used. Introducing the tiny neutrino masses, we have the following neutrino mass matrix for two heavy neutrinos (for a Dirac mass):

$$\begin{pmatrix} \mathcal{M}^{(3 \times 3)} & \mathcal{M}^{(2 \times 3)} \\ \mathcal{M}^{(2 \times 3)T} & \mathcal{M}^{(2 \times 2)} \end{pmatrix}, \quad (7.15)$$

where

$$\mathcal{M}^{(3 \times 3)} = \begin{pmatrix} m_{ee} & m_{e\mu} & m_{e\tau} \\ m_{\mu e} & m_{\mu\mu} & m_{\mu\tau} \\ m_{\tau e} & m_{\tau\mu} & m_{\tau\tau} \end{pmatrix}, \quad \mathcal{M}^{(2 \times 2)} = \begin{pmatrix} 0 & m_D \\ m_D & 0 \end{pmatrix}. \quad (7.16)$$

If N' does not mix with the neutrinos, i.e., if $\mathcal{M}^{(2 \times 3)} = 0$, it is truly sterile and must be decoupled at a very high temperature above 1 MeV by interactions beyond the SM. Most of these involve nonthermal production of N' [15]. One calculable case is the mixing of N' with light neutrinos in which case the neutrino oscillation converts some light neutrinos to some components of sterile neutrinos. Dodelson and Widrow [17] considered only one chirality of N' by introducing a tunable Majorana mass of N' , at a diagonal position of $\mathcal{M}^{(2 \times 2)}$ instead of the Dirac mass m_D in Eq. (7.16). The phenomenologically allowed abundance does not depend on the nature of Majorana or Dirac masses. The distinction resides in the symmetry argument. For the Dirac mass, we can use the above lepton number. For the Majorana mass, one just introduces a small parameter. Refining the calculation, the production rate is given by [17]

$$\Gamma = \frac{1}{2} \sin^2 2\theta_M \frac{7\pi}{24} G_F^2 T^4 E, \quad (7.17)$$

where the mixing angle $\sin 2\theta_M$ is temperature dependent due to matter effects in the plasma of finite temperature and density and expressed as [18]

$$\sin 2\theta_M \simeq \frac{\sin 2\theta}{1 + 0.08 \left(\frac{T}{100 \text{ MeV}} \right)^6 \left(\frac{\text{keV}^2}{\delta m^2} \right)}. \quad (7.18)$$

Here θ is the mixing angle in the vacuum where 0.08 is used for ν_μ and ν_τ mixing and is replaced by 0.27 for mixing with ν_e [19]. Due to the temperature dependence of the mixing angle and expansion rate, the maximum production rate to Hubble expansion takes place at a temperature [20, 21]

$$T \simeq 0.1 \text{ GeV} \left(\frac{m_s}{\text{MeV}} \right)^{1/3}. \quad (7.19)$$

The present relic density is estimated to be

$$\Omega_s \simeq 0.2 \text{ GeV} \left(\frac{\sin^2 \theta}{3 \times 10^{-9}} \right) \left(\frac{m_s}{3 \text{ keV}} \right)^{1.8}. \quad (7.20)$$

Thus, if the mass of the sterile neutrino is around keV, then they can become a realistic candidate for warm DM. The lifetime of sterile neutrino DM via three-body decay gives a constraint on the mixing angle. The decay into photon gives an even stronger bound on the mixing from X-ray observations as

$$\sin^2 2\theta < 2.5 \times 10^{-18} \left(\frac{0.86 \text{ MeV}}{m_s} \right). \quad (7.21)$$

At present, the original Dodelson–Widrow scenario seems in conflict with the X-ray observations.

Thus, the abundance of N' is a function of the N' mass and the mixing angles of N' with light neutrinos. The abundance calculation does not come from the

decoupling temperature of N' but by the amount of the oscillated neutrinos. The study allows sterile neutrinos with masses of several keV for cosmological DM.

Minimal dark matter

In the minimal dark matter (MDM) scenario, one extends the SM simply by adding one scalar n -tuple or one (vector-like) pair of spin-1/2 n -tuples of $SU(2)_L$ which may carry a weak hypercharge. It was named minimal [22] because only one n -plet is introduced with the known (gauge) interactions. For an n -tuple with hypercharge Y , for the scalar MDM or the fermionic MDM, let us represent them as

$$S_{\text{MDM}} = \begin{pmatrix} s_1 \\ s_2 \\ \vdots \\ s_n \end{pmatrix}_Y, \quad F_L^{\text{MDM}} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix}_{Y,L}, \quad F_R^{\text{MDM}} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix}_{Y,R}. \quad (7.22)$$

The neutral component of scalar S_{MDM} or fermion F^{MDM} is assumed to be the lightest component and is proposed to be a DM candidate. Stability of the lightest neutral member of the n -tuple is guaranteed by gauge symmetry and renormalizability; then, the minimality of the model gives definite predictions depending only on the mass M of the new matter states since the interaction mediators are determined by the gauge symmetry. The un-hypercharged elements of the new multiplets should obey the direct detection constraints.

For S_{MDM} , the quartic coupling of S_{MDM} reaches the Landow pole condition below the Planck scale for $n = 4, 5, 6, 7$ [23]. Thus, MDM with one scalar S_{MDM} is not allowed. The fully successful MDM candidates include a fermionic F^{MDM} with $n = 5$ and $Y = 0$. The phenomenological predictions and direct and indirect DM detections are well summarized in [24]. Since the MDM has electroweak interactions, the relic density can be naturally obtained via thermal freeze-out as for WIMPs [25] where coannihilation with slightly heavier elements of the multiplets ameliorates the result. The annihilation of MDM occurs dominantly through s -wave with subdominant effect of p -wave.

Strongly interacting massive particles

Another class of DM particles within the SM gauge group are known as strongly interacting massive particles (SIMPs) [26–29]. SIMPs might arise from gauge theories containing exotic stable heavy quarks, where the new heavy quarks are produced in the early Universe but later bind with lighter quarks to form neutral, massive, and strongly interacting particles. These types of SIMPs could be extremely massive, ranging far beyond the TeV scale. SIMPs may also arise in SUSY models where the gluino is the lightest SUSY particle [30]. Then gluinos produced thermally or nonthermally in the early Universe would bind with gluons to make a neutral gluino-balls which could comprise the DM. Gluino balls would be expected around the TeV

scale.² These types of SIMPs could give rise to exotic collider signatures such as charged stable tracks which flip charge as they propagate. Recently, a new SIMP paradigm was proposed [8] where DM arises from a secluded dark sector, discussed in Section 7.3.1, which is thermalized with the SM after reheating. These SIMPs could exist in the MeV–GeV range, depending on physics of the secluded sector. SIMPs can be identified as hidden pions in the hidden confinement sector, which are described by a nonlinear sigma model with an unbroken flavor symmetry, G/H . A hidden confining sector from string compactification is possible [124]. The unbroken flavor symmetry ensures the longevity of the pions. It has been shown that the kinetic interaction of SIMPs with the SM sector has a big impact on the relic density of DM [33].

The variety of production mechanisms and huge span of mass possibilities lead to great uncertainty in the SIMP production rate in the early Universe. However, since SIMPs are strongly interacting, it is often expected that they might bind to nuclei and so can be sought after in exotic, massive nuclei searches. Indeed, heavy relic techni-baryon DM particles seem ruled out by this approach [32].

Wimpzillas: Supermassive DM

Wimpzillas are very massive particles that cannot be produced thermally, since their mass M_{wz} is much larger than the reheating temperature itself. They however can be produced with mass of order the inflaton mass in the transition from inflation to the matter- or radiation-dominated Universes due to nonadiabatic expansion by classical gravitational effects [34, 35]. Independent of their couplings, Wimpzillas with mass in the range $0.4 \lesssim M_{\text{wz}}/H_I \lesssim 2$ (with the Hubble parameter at the end of inflation $H_I \simeq m_\phi \simeq 10^{13}$ GeV) can have the right relic density in the present Universe provided that they are stable [36, 37]. They can be produced non-thermally by nonperturbative quantum effects in preheating or by the collisions of vacuum bubbles in a first-order phase transition [38]. Supermassive particles can be produced also during reheating after inflation [39]. Since the maximum temperature after inflation is much higher than the reheating temperature, the Wimpzillas can be produced thermally from scatterings during the reheating process. In the slow reheating process, the analytic estimate for the relic density is [39]

$$\Omega h^2 \simeq M_{\text{wz}}^2 \langle \sigma v \rangle \left(\frac{200}{g_*} \right)^{3/2} \left(\frac{2000 T_{\text{reh}}}{M_{\text{wz}}} \right)^7. \quad (7.23)$$

7.3. Other massive particles

In this section, we discuss other candidates, which require a new confining force, or extra dimensions, or others arising irrespective of the decoupling temperature T_{dec} .

²With the invisible axion, the gluino mass can be as low as 800 GeV [31].

7.3.1. *With a new confining force*

DM can be a part of a multiplet of states with a new confining force [40]. The motivation for suggesting such a dark force was in view of the rise of cosmic electron flux above 100 GeV: for a 800 GeV DM particle to annihilate into leptons at a level well above that expected from a thermal relic. A comprehensive study from a new confining force has been also studied in [41].

With a new confining force, the DM density can come either from the calculation of the decoupling temperature or by a pre-assigned asymmetry as in the case of baryon number generation. These issues are studied in Chapters 2 and 8.

7.3.2. *Kaluza–Klein DM*

In models of universal extra dimensions (UED) [42], it is assumed that the SM particles exist in an extra-dimensional universe, but that the extra dimensions are compactified on some sort of topological manifold such that four-dimensional (4D) chiral representations are allowed. The well-known example is an orbifold compactification, allowing 4D SM [43–47]. Orbifolding eliminates unwanted wrong helicity modes, leaving just the chiral spectrum in the SM as the low energy effective theory.

In UED models, the SM particles exist as the $n = 0$ Kaluza–Klein (KK) modes, along with an infinite tower of their KK excitations $n = 1, 2, 3, \dots$. The $n = \text{even}$ KK modes, including the $n = 0$ mode, upon compactification have the wave function proportional to $\cos(ny/R)$ where y is the fifth dimension coordinate, see, for example, Ref. [47]. On the other hand, the $n = \text{odd}$ KK modes have the wave function proportional to $\sin(ny/R)$. These KK excitations, basically heavier copies of the SM particles with the same spin and couplings, have mass $m_{\text{KK}}^n \sim n/R$, where R is the compactification radius. These wave functions are parity (in the fifth coordinate) even and odd, respectively, which are called the KK parities. The $n = 0$ modes include the SM particles. All the KK parity odd particles are heavy. LHC searches now constrain $R^{-1} \gtrsim 1$ TeV. In UED models, KK parity is conserved wherein all $n = 1$ (excited state) particles decay to other $n = 1$ particles so that the lightest $n = 1$ particle is absolutely stable, and denoted as the lightest KK particle (LKP). The LKP can be a good DM candidate [48, 49]. Possibilities for LKP include the $n = 1$ KK photon, KK neutrino or KK graviton with mass $m_{\text{LKP}} = 1/R$. The photon or neutrino LKPs enjoy electroweak interactions with SM particles and hence become WIMPs. Their relic density is determined thermally via freeze-out from the thermal plasma and it is found that KK photons/neutrinos with mass ~ 1 TeV scale can account for the correct relic density [50–53]. Including coannihilation processes, then even lighter LKPs around 0.6–0.9 TeV are required. Projections for direct LKP-photon nucleon spin-independent scattering cross-sections still lie about an order of magnitude below recent LUX limits [54]. Even so, since one also expects a variety of $n = 1$ KK quark and lepton states around the 1 TeV scale, then in light of recent null results from LHC searches for new physics, the simplest UED

DM scenarios seem increasingly unlikely. If instead the KK graviton is the LKP, it interacts very weakly with SM particles and becomes an E-WIMP or super-WIMP [121] and can be produced from the decays of heavier KK excitations which would be present in the thermal plasma (care being taken to avoid Big Bang nucleosynthesis constraints). Alternatively, if the KK graviton is not LKP, then it can still be produced thermally but may contribute via decay to the nonthermal production of the LKP WIMPs [56]. The phenomenology of KK DM including discussion of direct and indirect searches and physics at colliders is reviewed in [57].

7.3.3. Branon

In models with extra spacetime dimensions, the brane where our world is located can move and fluctuate along the extra dimensions. In this case, there appears a new degree of freedom which parameterizes the position of the visible brane in the extra dimensions. When the metric is not warped along the extra dimensions, the transverse brane fluctuations, branons, can be parameterized by Goldstone boson associated to the spontaneous breaking of the extra-space translational symmetry and becomes massless [58]. As an example, for a single extra dimension of a circle with brane parameterization $Y^M = (x^\mu, y(x))$, the metric induced on the brane is

$$g_{\mu\nu} = \partial_\mu Y^M \partial_\nu Y^N G_{MN}. \quad (7.24)$$

With metric $G_{MN} = (\tilde{g}_{\mu\nu}, -1)$, the brane action can be written as

$$S_B = -f^4 \int_{M_4} d^4x \sqrt{g} \simeq -f^4 \int_{M_4} d^4x \sqrt{\tilde{g}} \left(1 - \frac{1}{2} \tilde{g}^{\mu\nu} \partial_\mu Y \partial_\nu Y \right), \quad (7.25)$$

where f is the brane tension. This Y is parameterized by the Goldstone boson. The warp factor breaks the translational symmetry explicitly and generates a mass m_b for the branons which is given by the bulk Riemann tensor evaluated at the brane position. Parity symmetry on the brane then requires branons to couple as pairs to the SM particles and then implies the branon stability so that they may serve as a DM candidate [59]. In a more general setup, the brane action is obtained up to quadratic terms as [60, 61]

$$S_B = \int_{M_4} d^4x \sqrt{\tilde{g}} \left[\frac{1}{2} (\tilde{g}^{\mu\nu} \delta_{\alpha\beta} \partial_\mu \pi^\alpha \partial_\nu \pi^\beta - M_{\alpha\beta}^2 \pi^\alpha \pi^\beta) \right. \quad (7.26)$$

$$\left. + \frac{1}{8f^2} (4\delta_{\alpha\beta} \partial_\mu \pi^\alpha \partial_\nu \pi^\beta - M_{\alpha\beta}^2 \pi^\alpha \pi^\beta) T_{\text{SM}}^{\mu\nu} \right], \quad (7.27)$$

where the branon field $\pi^\alpha(x) = f^2 \delta_m^\alpha Y^m(x)$ and their mass matrix is $M_{\alpha\beta}^2 = \tilde{g}^{\mu\nu} R_{\mu\alpha\nu\beta} \Big|_{y=0}$. The branons interact with the SM particles through their energy-momentum tensor with a coupling suppressed by the inverse of the brane tension scale f [58, 62–64]. In the case where f and m_b are $\sim m_{\text{weak}}$, then the branons behave like WIMPs and would give rise to CDM as usual via the WIMP miracle

scenario. Branons may interact with nuclei; thus giving direct WIMP detection signals, and they may annihilate into the SM particles giving indirect cosmic anti-matter and gamma ray signatures. The distinguishing characteristic of branons from other WIMPs (e.g., neutralinos of SUSY or KK photons from UED models) is that they could be produced directly at colliders giving rise to monojet or monophoton signatures, but without the additional cascade decay signatures expected from models like SUSY or UED.

7.3.4. *Chaplygin gas*

A perfect fluid with an equation of state given by

$$p = -\frac{A}{\rho} \quad (7.28)$$

is known as a Chaplygin gas. Here, p and ρ are pressure and energy density respectively with $\rho > 0$ and A is a positive constant. The Chaplygin equation of state can be obtained from the Nambu–Goto action for d-branes moving in a $(d + 2)$ -dimensional spacetime in the light-cone parameterization. This gas can be used to account for DM and DE simultaneously [65], and has been later connected to M-theory and brane models [66–69].

In the FLRW cosmology, the equation of state gives rise to a solution

$$\rho = \sqrt{A + \frac{B}{a^6}}, \quad (7.29)$$

where a is the scale factor and B is a constant of integration. In the limit of small a , then the energy density behaves as matter:

$$\rho = \frac{\sqrt{B}}{a^3}, \quad (7.30)$$

while for large a then the energy density is

$$\rho = \sqrt{A}, \quad \text{while } p = -\sqrt{A}, \quad (7.31)$$

i.e., the cosmological constant is $\Lambda_{\text{cc}} = \sqrt{A}$.

The generalized Chaplygin gas model was further considered in [70]. These models seem to have tension with both structure formation [71] and CMB [72, 73]. So, further modified models have been considered.

7.3.5. *Primordial black hole*

When primordial density perturbations are large, of order unity on the scale of the cosmological horizon, in the early Universe, primordial black holes (PBHs) can form

[74]. The lifetime of a PBH is connected to its mass due to Hawking radiation as [74, 75]

$$\tau_{\text{PBH}} \simeq 10^{64} \left(\frac{M_{\text{PBH}}}{M_{\odot}} \right)^3 \text{ years}, \quad (7.32)$$

where $M_{\odot} = 2 \cdot 10^{33} \text{ g}$ is the Sun's mass. In this case, the PBH has survived until now if the PBH mass is sufficiently small, $M_{\text{PBH}} < 10^{15} \text{ g}$.

The large primordial density perturbations can be generated during inflation. However, the power law spectrum from inflation gives too small a PBH density or else it is constrained by the photons evaporated [76]. Therefore, a spectrum with special feature at some characteristic scale has been suggested to be a dominant DM component [77]. The PBH can be formed also from phase transitions [78, 79], collapse of the string loops, bubble collisions, or collapse of domain walls [80].

Some recent claims exist [81, 82] which seem to exclude PBHs as DM due to the possibility that they would bind with and subsequently swallow neutron stars although these studies have been called into question due to overly optimistic assumptions about the abundance of DM in globular clusters or on the PBH–neutron star capture rate. Other studies using data from the Kepler satellite have looked for planetary level microlensing effects and found no candidate events. This has allowed a substantial range of $M_{\text{PBH}} < 10^{-9} - 10^{-7} M_{\odot}$ to be excluded for a large enough PBH halo fraction [83]. In the case where PBHs coexist with WIMP DM, then it is claimed that the PBH will form an ultra-compact mini halo of DM around itself which will serve as an intense γ -ray point source due to WIMP–WIMP annihilations [84]. Constraints from γ -ray searches seem to rule out this possibility. If we accept all these constraints, the allowed mass bound of PBH is

$$M_{\text{PBH}} \lesssim 10^{-7} M_{\odot}. \quad (7.33)$$

7.3.6. *Asymmetric dark matter*

The asymmetric dark matter (ADM) will be discussed in the subsequent chapter where the baryon asymmetry is also discussed.

7.3.7. *Extremely-weakly interacting massive particles*

Beyond the WIMPs, we can consider extremely-weakly interacting massive particles (E-WIMPs). Depending on the physical and cosmological properties, in the literature these are named as axinos [85], super-weakly interacting massive particles (SWIMPs) [86], and feebly interacting massive particles (FIMPs) [87]. Obviously, the axino is the superpartner of axion with the spontaneously broken $U(1)_{\text{PQ}}$ symmetry. Thus, the interaction scale of axino is the axion decay constant f_a . The typical interaction strength of the other E-WIMPs are the Planck mass M_{P} or the GUT scale M_{GUT} . SWIMPs are supposed to be produced by the WIMP decay after

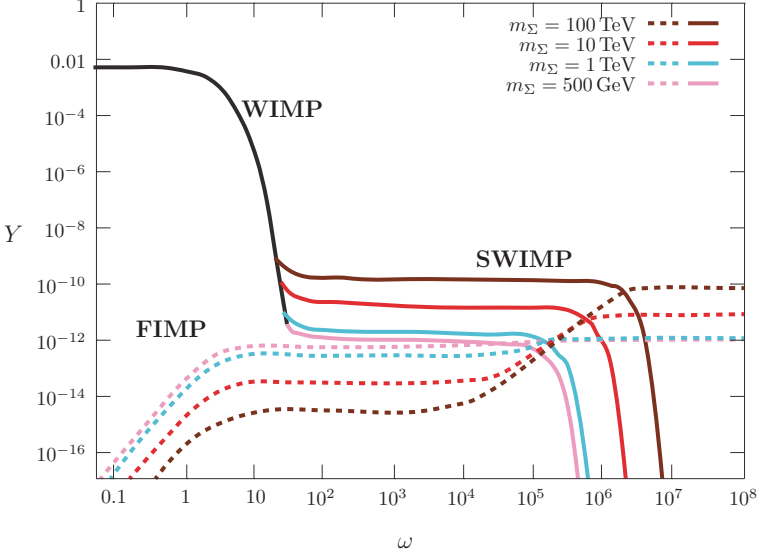


Fig. 7.5. E-WIMP abundances [88]. SWIMPs are on the RHS marked with solid lines, which are generated by the WIMP decay. FIMP abundances are shown as dashed curves. Y is the yield of DM, and $\omega = m_\Sigma/T$. The axino mass is set at 100 GeV and typical Yukawa couplings are chosen as 10^{-12} .

freeze-out. Two well-known examples of SWIMPs are “gravitino” and KK graviton. FIMPs are supposed to be produced even during the equilibrium state of the WIMP.

In Fig. 7.5, we present a numerical study for an example which can cover both SWIMP and FIMP scenarios. These depend on the model parameters such as ω . For the gravitino SWIMP, an interesting scenario for the ratio of $\rho_{\text{DM}}/\rho_B \approx 5$ has been suggested in an R -parity violating SUSY model [89].

“Freeze-out” is defined as usual when the number density is frozen after certain cosmic time scale. In Fig. 7.5, these are shown on the RHS of the WIMP decay time. “Freeze-in” is defined when the number density is growing even when the WIMPs are in thermal equilibrium [87], which occurs when the reheating temperature is higher than the mass of the freezein particle

$$m < T_{\text{reheat, SM}}, \quad (7.34)$$

where the temperature on the RHS is calculated with the SM particles only. It is shown that the mass fraction is independent of the freezein mass m [90],

$$m Y_{\text{freeze in}} = m \lambda^2 \left(\frac{M_{\text{P}}}{m} \right) \sim \lambda^2 M_{\text{P}}, \quad (7.35)$$

where λ is a coupling constant. Freezein particles have never been in equilibrium in the whole history of the Universe. These are on the LHS of the WIMP equilibrium

curve, showing that even when WIMP is still living, E-WIMPS are created starting from nothing.

In the remainder of this chapter, we discuss two E-WIMP examples, axino and gravitino.

7.4. Axinos

A discrete subgroup of gauge $U(1)$ s and R -parity are two important applications of discrete symmetries. If R -parity quantum numbers of SM particles are given by $3B - L + 2S$, such an R -parity is not exact because it contains global charges B and L which must be approximate. If R -parity is defined as a discrete subgroup of $U(1)_R$ global symmetry, which is better to be called “matter parity” [7], the R -parity is approximate because global symmetries are not respected by gravity. The approximate nature of the Peccei–Quinn (PQ) symmetry $U(1)_{PQ}$ and $U(1)_R$ global symmetry has been shown explicitly in obtaining the MSSM from the orbifold compactification [91, 92].

Figure 4.5 shows how an approximate global symmetry is obtained from a top-down approach. As discussed in Section 6.6, gauge and discrete symmetries are not spoiled by gravity but global symmetries are spoiled by gravity.

One can consider a series of interaction terms allowed by the discrete symmetry. The vertical red of Fig. 4.5 shows the infinite tower of terms, not spoiled by gravity. If one considers the few lowest order terms of the red column, there can be an accidental global symmetry. With this global symmetry, one can consider an infinite series of terms shown as the horizontal green of Fig. 4.5. The terms shown in lavender satisfy both of these discrete and global symmetry conditions. But, the horizontal green terms outside the lavender do not satisfy the discrete symmetry and the global symmetry is spoiled by gravity. The vertical red part terms not spoiled by gravity give the global symmetry braking terms. Thus, there results an approximate global symmetry [93–95].

Axino $\tilde{a}$ seems to be defined by the global symmetry $U(1)_{PQ}$, as the ϑ component of the axion supermultiplet A (in two-component notation),

$$A = \frac{1}{\sqrt{2}}(s + ia) + \sqrt{2}\tilde{a}\vartheta + F_A\vartheta\vartheta, \quad (7.36)$$

where F_A stands for an auxiliary field of A and ϑ is the Grassmann superspace anticommuting coordinate, as introduced in Section 4.8. But, axion and hence axino also are defined below the scale where the $U(1)_{PQ}$ is spontaneously broken. If we consider the global SUSY, Eq. (7.36) is a proper definition of axino. Indeed, in early days of axino, the above definition has been used to observe some physical effects on axino interactions when its mass is small [96–104]. At the EW scale, a proper implementation of SUSY is the local SUSY, i.e., supergravity, where one considers spontaneously broken local SUSY. For the intermediate scale axion decay constant, spontaneous breaking of supergravity and $U(1)_{PQ}$ can be comparable as

suggested in [105]. Then, one must consider gravitino together with axino. The importance of this consideration is conspicuous when axino mass is around the electroweak scale [104, 106], and a proper definition of axino in spontaneously broken supergravity has been given in [107]. In supergravity, there remain viervein e_μ^a ($S_z = \pm 2$) and gravitino ψ_μ ($S_z = \pm \frac{3}{2}$) after satisfying all constraints. The local SUSY transformation parameter for the Lorentz index a is $\xi^a = 2i(\vartheta\sigma^a\bar{\zeta}(x) - \zeta(x)\sigma^a\bar{\vartheta})$ with a spinor parameter ζ carrying the x -dependence while keeping ϑ independent of x . Then, the SUSY transformation changes viervein to gravitino [108],

$$\delta e_\mu^a = i(\psi_\mu\sigma^a\bar{\zeta}(x) - \zeta(x)\sigma^a\bar{\psi}_\mu). \quad (7.37)$$

When the local SUSY is spontaneously broken, then the gravitino components ($S_z = \pm \frac{3}{2}$ components) are completely filled by the addition of the goldstino ($S_z = \pm \frac{1}{2}$ components), and gravitino becomes massive. Its mass is proportional to the SUSY breaking scale “ F -term”/ $\sqrt{3}M_P$ [109]. So, in the definition of the massive gravitino, it is important to know how the SUSY breaking is inserted. For simplicity, we consider only the F -term breaking of SUSY. If there are many chiral fields developing F -terms, the overall factor is the one contributing to the SUSY breaking,³

$$F = \sqrt{\sum_i F^i F_i}, \quad (7.38)$$

where F_i is the F component of the chiral field i . The massive gravitino $\tilde{G}$ is ψ_μ plus $g_{1/2}$ (= goldstino), which is depicted in Fig. 7.6.

If we introduce only one chiral field which breaks both $U(1)_{PQ}$ and SUSY, then there is no axino, or goldstino corresponds to axino. But, let us not interpret goldstino as axino and define axino such that it is orthogonal to goldstino. To introduce

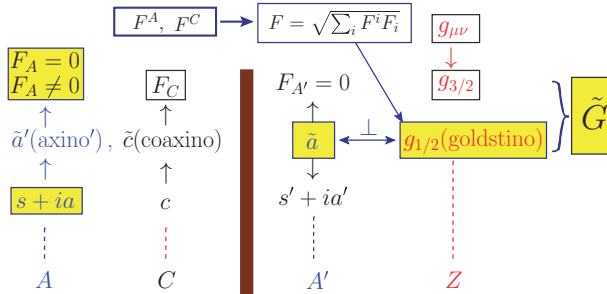


Fig. 7.6. The axion (blue) and goldstino (red) multiplets [107]. The axion direction a is defined by the PQ symmetry, and the goldstino ($g_{1/2}$) and axino ($\tilde{a}$) directions are defined by the orthogonality in the $S_z = \frac{1}{2}$ fermion mass matrix as shown in the figure.

³If SUSY is broken by a D -term, F may be defined as $\sqrt{D}$.

axino, then we must introduce at least two chiral fields, which has been studied in Ref. [107].

In the most general framework, including the nonminimal Kähler potential, the axino mass can be studied [107], where the axino mass is given by $m_{\tilde{a}} = m_{3/2}$ for $G_A = 0$, where $G = K + \ln|W|^2$ with $G_A \equiv \partial G/\partial A$. For $G_A \neq 0$, the axino mass depends on the details of the Kähler potential. In the gauge mediation scenario, the gaugino mass is the dominant axino mass parameter. In the case of gravity mediation, the axino mass is likely to be greater than the gravitino mass, but one cannot rule out lighter axinos [107].

SUSY models of very light axion can provide a clue about the magnitude of the axion decay constant f_a . In Refs. [14, 105], it was speculated that f_a is related to the MSSM Higgs/higgsino mass parameter μ as $f_a \sim \sqrt{\mu M_P}$. To avoid gravity spoil of global symmetries to the required level, viz. Section 6.6, f_a has been given from string inspired discrete symmetries such as $S_2 \times S_2$ symmetry [110].

In fact, the most important axino parameter in cosmological considerations, the axino mass $m_{\tilde{a}}$, does not even appear in Eq. (7.48) which will be presented later. SUSY breaking generates the masses for the axino and the saxion and modifies their definitions. The saxion mass is set by the SUSY soft breaking mass scale, M_{SUSY} [97, 111]. The axino mass, on the other hand, is strongly model dependent. An explicit axino mass model with SUSY breaking was first constructed long time ago [105] with the superpotential W with the PQ symmetry transformation $S \rightarrow e^{i\alpha} S$ and $\bar{S} \rightarrow e^{-i\alpha} \bar{S}$,

$$W = \sum_{i=1}^{n_I} Z_i (S\bar{S} - f_i^2), \quad n_I \geq 2. \quad (7.39)$$

With $n_I = 1$, the $U(1)_{\text{PQ}}$ symmetry is spontaneously broken, but SUSY remains unbroken. The case $n_I = 2$ breaks SUSY, which however gives $m_{\tilde{a}} = 0$ [105].

As first pointed out by Tamvakis and Wyler [97], the axino mass is expected to receive at least a contribution on the order of $m_{\tilde{a}} \sim \mathcal{O}(M_{\text{SUSY}}^2/f_a)$ at the tree level in the spontaneously broken global SUSY. In the literature, a whole range of axino mass was considered; in fact it can be even much smaller [98–101, 104], or much larger, than the magnitude of M_{SUSY} [106]. Because of this strong model dependence, in cosmological studies one often assumes axino interactions as given by the $U(1)_{\text{PQ}}$ symmetry and treats the axino mass as a free parameter.

One lucid, but often overlooked, aspect of the axino is that its definition must be given at a mass eigenstate level. The coupling to the QCD sector given in the first line of Eq. (7.48) can plausibly be that of the axino, but it does not give the axino mass. As already commented above, axino is connected to two kinds of symmetry breaking: the PQ global symmetry breaking and the SUSY breaking. These, in general, are not orthogonal to each other. The PQ symmetry breaking produces an almost massless pseudo-Goldstone boson (axion), while SUSY breaking produces massless goldstino. The massless goldstino is then absorbed into the gravitino to make it heavy via the super-Higgs mechanism.

Even though its name refers to the axion-related QCD anomaly, one must select the component that is orthogonal to the goldstino. If there are two SM singlet chiral fields, this is simple because there is only one component left beyond the goldstino. However, if more than two chiral fields are involved in SUSY breaking, more care is needed to identify the orthogonal mass eigenstate. Among the remaining mass eigenstates beyond the goldstino, a plausible choice for the axino field is the component whose coupling to the QCD anomaly term is the biggest. For two initial chiral fields in Fig. 7.6, $\tilde{a}'$ has the anomaly coupling of Eq. (7.48); hence, the $\tilde{a}$ coupling to the QCD sector is equal to or smaller than those given in Eq. (7.48). The remaining coupling is the one to the $s = \pm\frac{1}{2}$ components of a massive gravitino. Therefore, for the two initial chiral fields, axino cosmology must include the gravitino as well, if $\tilde{a}'$ is not identical to $\tilde{a}$. The “leakage” is parameterized by the F -term of the initial axion multiplet A . With more than two initial chiral fields, the situation involves more mass parameters. One notable corollary of Ref. [107] is that the axino CDM relic abundance for $m_{\tilde{a}} < m_{3/2}$ is an overestimate if A obtains the F -term.

To write down the axino interaction with TeV scale SUSY particles, here we include the axion interaction with W and Z bosons also,

$$\begin{aligned} \mathcal{L}_{\text{SM gauge bosons}} = & \frac{1}{2} \partial^\mu a \partial_\mu a + (c_2 + c_3) \frac{a}{32\pi^2 f_a} g_3^2 G_{\mu\nu}^a \tilde{G}^{a\mu\nu} \text{ (or } \mathcal{L}_{\text{det}}) \\ & + \frac{a}{32\pi^2 f_a} \left(g_2^2 W_{\mu\nu}^a \tilde{W}^{b\mu\nu} (\text{Tr } T_a T_b) + g'^2 Y_{\mu\nu} \tilde{Y}^{\mu\nu} (\text{Tr } Y_L^2 + \text{Tr } Y_R^2) \right), \end{aligned} \quad (7.40)$$

where the coefficients of the axion and SU(2)- and U(1)_Y-anomaly couplings, $W_{\mu\nu}^a \tilde{W}^{a\mu\nu}$ and $Y_{\mu\nu} \tilde{Y}^{\mu\nu}$, are usually denoted as c_{aWW} and c_{aYY} , respectively, which depend on the models.

Example 7.1 (Pseudoscalar–gauge boson couplings). As the simplest example without coupling to gluons, let us introduce a vector-like doublet with the hypercharge $Y = -\frac{1}{2}$,

$$\ell_L = \begin{pmatrix} N \\ E \end{pmatrix}_L, \quad \ell_R = \begin{pmatrix} N \\ E \end{pmatrix}_R. \quad (7.41)$$

Let us also introduce SU(2)×U(1) singlets,

$$S, \quad \text{with a GUT-scale VEV } M_{\text{GUT}}, \text{ but not breaking } \text{U}(1)_{\text{global}}, \quad (7.42)$$

$$\sigma, \quad \text{with a VEV } f/\sqrt{2}, \text{ breaking } \text{U}(1)_{\text{global}}. \quad (7.43)$$

In the SM, the pseudoscalar coupling to color singlet gauge bosons is

$$\mathcal{L} = \frac{P}{f} \frac{g_2^2}{32\pi^2} W_{\mu\nu}^a \tilde{W}^{b\mu\nu} (\text{Tr } T_a T_b) + \frac{P}{f} \frac{g'^2}{32\pi^2} Y_{\mu\nu} \tilde{Y}^{\mu\nu} (\text{Tr } Y_L^2 + \text{Tr } Y_R^2), \quad (7.44)$$

Table 7.2. Quantum numbers of some U(1).

	ℓ_L	ℓ_R	σ	S
$\mathbf{Z}_{12}$	-1	+1	2	4
Q	-1	+1	2	4

where $W_{\mu\nu}^a$ is the non-Abelian field strength of SU(2) gauge fields A_μ^a , and $Y_{\mu\nu}$ is the U(1) field strength of U(1)' gauge fields Y_μ , and P is the phase field of σ , $\langle\sigma\rangle = \frac{f+p}{\sqrt{2}}e^{iP/f}$. For a vector-like fundamental representation in SU(N), like a heavy quark axion model or Eq. (7.41), $\text{Tr } T_a T_b = \delta_{ab}$. In Table 7.2, we present the $\mathbf{Z}_{12}$ discrete quantum numbers of σ and S together with the quantum numbers of an approximate U(1) $_Q$. Thus, Eq. (7.44) becomes

$$\begin{aligned}
\mathcal{L} &= \frac{P}{f} \frac{g_2^2}{32\pi^2} W_{\mu\nu}^a \tilde{W}^{a\mu\nu} + \frac{P}{f} \frac{g'^2}{32\pi^2} Y_{\mu\nu} \tilde{Y}^{\mu\nu} \\
&= \frac{P}{32\pi^2 f} \left(2g_2^2 W_{\mu\nu}^+ \tilde{W}^{-\mu\nu} + g_2^2 (1/c_W^2 - 2s_W^2) Z_{\mu\nu} \tilde{Z}^{\mu\nu} \right. \\
&\quad \left. + 2e^2 F_{\mu\nu}^{\text{em}} \tilde{F}^{\text{em}\mu\nu} + 2eg_2 c_W F_{\mu\nu}^{\text{em}} \tilde{Z}^{\mu\nu} \right), \tag{7.45}
\end{aligned}$$

where

$$\begin{aligned}
W_\mu^3 &= \cos\theta_W Z_\mu + \sin\theta_W A_\mu, \\
Y_\mu &= -\sin\theta_W Z_\mu + \cos\theta_W A_\mu, \\
c_W &= \cos\theta_W = \frac{g_2}{\sqrt{g_2^2 + g'^2}}, \\
s_W &= \sin\theta_W = \frac{g'}{\sqrt{g_2^2 + g'^2}}.
\end{aligned}$$

Thus, the massless combination to the photon coupling is parameterized by $c_{P\gamma\gamma}$,

$$\mathcal{L}_{P\gamma\gamma} = \frac{c_{P\gamma\gamma} P}{f} \frac{e^2}{32\pi^2} F_{\mu\nu}^{\text{em}} \tilde{F}^{\text{em}\mu\nu}, \tag{7.46}$$

where $c_{P\gamma\gamma}$ from Eq. (7.41) turns out to be 2.

In particular, the interaction of the axion supermultiplet A with the vector multiplet V_a , which is a SUSY version of the c_3 term in Eq. (7.40), is given by

$$\mathcal{L}^{\text{eff}} = - \sum_V \frac{\alpha_V C_{aVV}}{2\sqrt{2}\pi f_a} \int A \text{Tr} [V_a V^a] + \text{h.c.}, \tag{7.47}$$

where α_V denotes a gauge coupling, C_{aVV} is a model-dependent constant and the sum is over the SM gauge groups. From this, the relevant axino–gaugino–gauge-boson and axino–gaugino–sfermion–sfermion interaction terms can be derived and

are given by [112] (in four component spinor notation)

$$\begin{aligned}
\mathcal{L}_{\tilde{a}}^{\text{eff}} = & i \frac{\alpha_s}{16\pi f_a} \bar{\tilde{a}} \gamma_5 [\gamma^\mu, \gamma^\nu] \tilde{G}^b G_{\mu\nu}^b + \frac{\alpha_s}{4\pi f_a} \bar{\tilde{a}} \tilde{g}^a \sum_{\tilde{q}} g_s \tilde{q}^* T^a \tilde{q} \\
& + i \frac{\alpha_2 C_{aWW}}{16\pi f_a} \bar{\tilde{a}} \gamma_5 [\gamma^\mu, \gamma^\nu] \tilde{W}^b W_{\mu\nu}^b + \frac{\alpha_2}{4\pi f_a} \bar{\tilde{a}} \tilde{W}^a \sum_{\tilde{f}_D} g_2 \tilde{f}_D^* T^a \tilde{f}_D \\
& + i \frac{\alpha_Y C_{aYY}}{16\pi f_a} \bar{\tilde{a}} \gamma_5 [\gamma^\mu, \gamma^\nu] \tilde{Y} Y_{\mu\nu} + \frac{\alpha_Y}{4\pi f_a} \bar{\tilde{a}} \tilde{Y} \sum_{\tilde{f}} g_Y \tilde{f}^* Q_Y \tilde{f}, \tag{7.48}
\end{aligned}$$

where the terms proportional to α_2 correspond to the $\text{SU}(2)_L$ and the ones proportional to α_Y to the $\text{U}(1)_Y$ gauge groups, respectively. C_{aWW} and C_{aYY} are model-dependent couplings for the $\text{SU}(2)_L$ and the $\text{U}(1)_Y$ gauge group axino–gaugino–gauge-boson anomaly interactions, respectively, which are defined after the standard normalization of f_a , as in Eq. (7.40) for the $\text{SU}(3)_c$ term. Here, α_2 , $\tilde{W}$, $W_{\mu\nu}$ and α_Y , $\tilde{Y}$, $Y_{\mu\nu}$ are, respectively, the gauge coupling, the gaugino field and the field strength of the $\text{SU}(2)_L$, and the $\text{U}(1)_Y$ gauge groups. $\tilde{f}_D$ represents the sfermions of the $\text{SU}(2)_L$ doublet, and $\tilde{f}$ denotes the sfermions carrying the $\text{U}(1)_Y$ charge.

Similarly, one can derive supersymmetrized interactions of the axion supermultiplet with a matter multiplet as a generalization of the c_1 and the c_2 terms in Eq. (7.40). Reference [113] considered a generic form of the effective interactions and clarified the issue of the energy-scale dependence of axino interactions. At some energy scale p , which is larger than the mass of the PQ-charged and gauge-charged multiplet M_Φ , the axino–gaugino–gauge-boson interaction is suppressed by M_Φ^2/p^2 . This suppression is manifest in the DFSZ axion model, and even in the KSVZ model, if the heavy quark mass is relatively low compared to the PQ scale, in which case, of course, the heavy quark is not integrated out.

7.5. Gravitino

If SUSY is inevitable for a solution of the hierarchy problem, gravitino is another well-motivated E-WIMP.

A possibility for light gravitino DM was considered as relativistic thermal relics whose energy density is given by [114, 115],

$$\Omega_{3/2} h^2 \sim 0.1 \left(\frac{m_{3/2}}{0.1 \text{ keV}} \right) \left(\frac{g_*}{106.75} \right)^{-1}. \tag{7.49}$$

There also exists a possibility that the light gravitinos are decay products of axinos in the gauge-mediated SUSY breaking scenario [116]. A more popular example is the CDM possibility of gravitinos where gravitino is the LSP. Assuming the domination of the goldstino component in the gravitino production in the thermal bath, one

obtains [117–119],

$$\Omega_{3/2} h^2 \sim 0.03 \left(\frac{m_{3/2}}{0.1 \text{ GeV}} \right)^{-1} \left(\frac{T_{\text{reh}}}{10^9 \text{ GeV}} \right) \sum_i c_i \left(\frac{M_i}{100 \text{ GeV}} \right)^2, \quad (7.50)$$

where c_i are coefficients of $\mathcal{O}(1)$, M_i are the three gaugino masses at the electroweak scale and T_{reh} is the reheating temperature in supergravity in the range $\leq 10^9 \text{ GeV}$ [120]. In many cases, the gravitino population depends mostly as the decay products of the next-LSP (NLSP). This process called super-WIMP mechanism gives [121],

$$\Omega_{3/2} h^2 = \left(\frac{m_{3/2}}{m_{\text{WIMP}}} \right) \Omega_{\text{WIMP}} h^2, \quad (7.51)$$

where the NLSP is assumed to be a WIMP. Equations (7.50) and (7.51) provide the most popular scenarios of CDM gravitino in the gravitino mass range of $m_{3/2} = 1 \text{ GeV} - 1 \text{ TeV}$. It is reviewed in [122] and some of the LHC exclusion plot is already presented in Ref. [123].

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Chapter 8

Baryogenesis and ADM

Without memory there can be no insight — Anne Rice

The origin of the baryon asymmetry of the Universe (BAU) has been a longstanding theoretical issue. The baryon number density $n_B/n_\gamma \simeq 6.1 \times 10^{-10}$ is one of the most accurately determined quantity in the precision cosmology, as sketched in Chapter 2. At the cosmic temperature above 1 GeV, numbers of baryons and antibaryons must be comparable to that of photons. But the present value of n_B/n_γ is extremely small $O(10^{-9})$, implying a scenario that the Universe has started with the net baryon number almost zero before the nucleosynthesis era,

$$\Delta B \equiv \frac{n_B - n_{\bar{B}}}{n_\gamma} \simeq 0, \quad \text{at } t \ll 1 \text{ s.} \quad (8.1)$$

If indeed the Universe started with $\Delta B = 0$ at the time of CDM density determined in Fig. 1.3, there is a question, “How can one generate a nonzero net baryon number starting from an initial $\Delta B = 0$ Universe?” This is the so-called *baryogenesis* problem. As discussed in Chapter 2, three physical conditions of Sakharov are the key [1]:

- (i) There must be interactions with microscopic violation of baryon number.
- (ii) These interactions violate C and CP symmetries.
- (iii) These processes occur out of thermal equilibrium.

In fact, the first and the second conditions are important problems in particle physics. In this chapter, we discuss theories on creating global quantum numbers toward baryogenesis which are then applied to theories on asymmetric dark matter (ADM).

Regarding (i), the first obvious models were based on grand unified theories (GUTs) [2] where $\Delta B \neq 0$ interactions are present. Regarding (ii), at the level of the standard model (SM) of particle physics, there are two CP phases, one the

Cabibbo–Kobayashi–Maskawa (CKM) phase δ_{CKM} in the quark sector [3, 4] and the other the Pontecorvo–Maki–Nakagawa–Sakada (PMNS) phase δ_{PMNS} in the lepton sector [5], already presented in Section 4.7. These parameterizations are discussed in [4–9].¹ So, from the early time on, it has been an interesting issue to investigate a possibility of relating the baryon asymmetry ΔB with the SM phase(s) δ_{CKM} or/and δ_{PMNS} . The first obvious investigation was looking for a possibility of δ_{CKM} whether it works for the BAU or not. But, it has been known that δ_{CKM} is not enough for the baryon number generation suggested in GUTs [10].

The sphaleron process is effective during the electroweak (EW) phase transition [11]. The corresponding effective interaction is to change the chiralities of SU(2) doublets [12]. Change of chiralities is needed for nonzero ΔB in the sphaleron related processes. This process violates both baryon (B) and lepton (L) numbers, but conserves the baryon minus lepton number ($B - L$). If baryon number generation at a GUT scale occurred with the conserved $B - L$ as in the SU(5) GUT, all baryon numbers combine with all lepton numbers to make $\Delta B = \Delta L = 0$ (if the sphalerons are 100 % effective) during the EW phase transition. Therefore, baryogenesis or leptogenesis above the EW scale must have occurred with $B - L$ violating interaction(s). If any GUT is responsible for this, the GUT must be beyond SU(5).

There are more ideas for baryogenesis which will be briefly sketched in Section 8.1. In Section 8.2, creation of global quantum numbers will be discussed, which will be used in considering the ADM in Section 8.3.

8.1. Theories on baryogenesis

Creation of baryons is through heavy particle decay, scattering, and phase transition. Most widely used baryogenesis is to use the heavy particle decay, which implements Sakharov’s third nonequilibrium condition in the evolving Universe. Furthermore, the heavy particle decays can be classified into two broad categories: two or more decay channels and the phase transitions.

8.1.1. *GUT baryogenesis and leptogenesis*

Around the late 1960s when Sakharov suggested the idea of baryogenesis, $\Delta B \neq 0$ interactions were hard to figure out, when the fundamental interactions just above the nuclear physics scales were not known. After the discoveries of weak neutral current and asymptotic freedom, the EW theory has emerged as the model describing physics up to 100 GeV scale. But, the baryon number B is not violated in the SM.

¹The CKM parameterizations occur in many forms [4, 6, 7]. These parameterizations discussed in Section 4.7 are equivalent, but the CKM phases can be distinguished now with the accurately determined real angles. Parameterizations [4, 7] give $\delta_{\text{CKM}} = \alpha$, and [6] gives $\delta_{\text{CKM}} = \gamma$ [8] where α, β, γ are three angles in the unitary triangle, summarized in [9].

The baryon number violating interaction appeared in GUTs, unifying strong, electromagnetic, and weak forces of the SM. Then, proton decay has been considered to be the most important prediction of GUTs [13]. The $\Delta B (= B_{\text{initial}} - B_{\text{final}})$ nonzero processes in GUTs have been appreciated in 1978 [2] since the Big Bang nucleosynthesis (BBN) was firmly accepted after 1977 [14, 15]. Departures from thermal equilibrium occur in an expanding Universe, possibly satisfying Sakharov's third condition. A significant $\Delta B \neq 0$ is difficult to be realized by scattering processes at a GUT temperature since the scattering of ordinary (i.e., effectively massless) fermions processes have no mass threshold as pointed out by Toussaint, Treiman, Wilczek, and Zee [16]. But, it was shown that the decay of a heavy X could produce an appropriate ΔB as the temperature T falls below the mass M_X . Then, this does not belong to the class of the thermal production but to the class of nonthermal production of ΔB . Furthermore, if the decay products are the SM fermions where the CP phase is provided by the CKM matrix, a calculation shows that $\Delta B \approx 10^{-18}$ [10]. Thus, a GUT scenario for ΔB generation has moved for the decaying scalar case: X decaying to particles carrying nonzero baryon numbers.

The GUT baryogenesis [2], leptogenesis [17], and “Q-genesis” [18] employ the above method of heavy particle decay. If there is only one decay channel, nonzero baryon number cannot be generated by the decay of a heavy particle. In this kind of baryon number generation in the Universe, we must introduce the same number of particles and antiparticles of the decaying species, say X , in the beginning, $\Delta N_{\text{initial}}^X = N_{\text{initial}}^X - N_{\text{initial}}^{\bar{X}} = 0$. If there is only one $\Delta B \neq 0$ channel, the particle X decay produces $B = a$ and its antiparticle $\bar{X}$ decay will produce $B = -a$; thus if there is only one decay channel, then there will be no net nonzero ΔB generated.

This GUT scale generation of ΔB went into another twist because of the QCD instanton process, violating the baryon number [12]. Applying this to $SU(2)_L$ weak sphaleron processes, one expects that baryon number violation, but with baryon minus lepton number ($B - L$) conservation, occurred at the EW phase transition in the evolving Universe [11]. The sphaleron process, changing the chiralities, conserves $B - L$ as shown in Fig. 8.1. Therefore, even if ΔB were generated at a GUT scale, it might be erased during the EW phase transition. Since $B - L$ is conserved, generation of lepton number L at a high energy scale was suggested [17]. Then, during the EW phase transition some L is converted to B via the process that conserves $B - L$. This is the so-called *leptogenesis*. Yet, another mechanism for baryogenesis above the EW scale called “Q-genesis”, innocent of the EW phase transition, has been also suggested [18].

Recently, the leptogenesis mechanism got most interest, which will be discussed more in Section 8.2.

8.1.2. Electroweak baryogenesis

There is a method that employs scattering instead of a heavy particle decay. It is the electroweak baryogenesis (EWBG) which uses the interaction of nine quark and

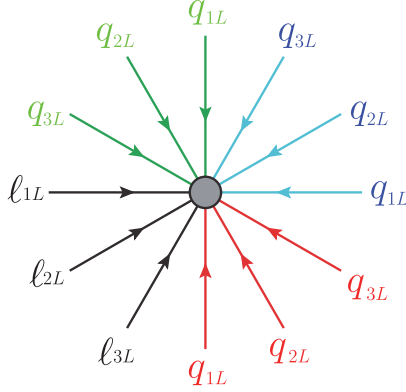


Fig. 8.1. The sphaleron process, conserving $B - L$. Here, q_i and ℓ_i are the i th family quark and lepton doublets.

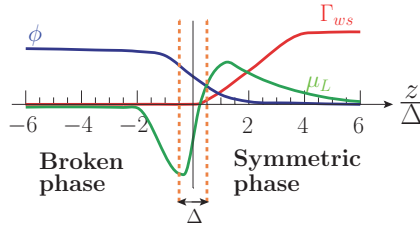


Fig. 8.2. Sketches of the scalar profile, the sphaleron rate and the chemical potential.

three lepton doublets during the EW phase transition epoch [11, 19]. This sphaleron generated effective interaction is effective when the temperature of the Universe was at the EW scale.

The EWBG [11] employs the sphaleron processes, as shown in Fig. 8.1, to have $\Delta B \neq 0$ and CP violation.² Cosmologically, this is realized through the phase transition at the boundary of two phases (of $SU(2) \times U(1)_Y$ preserving and $SU(2)_L \times U(1)_Y$ breaking vacua). These two phases having different B numbers must be well separated, and a sphaleron domain wall exists between them. Around the wall of thickness Δ , the profiles for scalar ϕ , the sphaleron rate Γ , and the chemical potential μ_L are sketched in Fig. 8.2, and the baryon asymmetry is expressed in the form, e.g., [21],

$$\eta_B = \frac{n_B(-\infty)}{s} = \frac{135N_c}{4\pi^2 v_{\text{ew}} g^* T} \int_{-\infty}^{\infty} dz \Gamma_{ws} \mu_L \exp \left[-\frac{3}{2} A \frac{1}{v_{\text{ew}}} \int_{-\infty}^z dz_0 \Gamma_{ws} \right],$$

²The sphaleron interaction changing chirality is violating P and hence violating CP. The QCD angle θ_{QCD} and the CKM phase δ_{CKM} have been also used [20, 25].

where s is the entropy, N_c is the number of colors, z is the direction orthogonal to the sphaleron surface, A is the sphaleron area at z , and

$$\Gamma_{ws} = 10^{-6} T e^{-\frac{E_{\text{sph}}}{T} \frac{\phi(T)}{v_{\text{ew}}}} \quad \text{with } E_{\text{sph}} \simeq 0.73\pi \frac{v_{\text{ew}}}{e} [22].$$

The phase transition in the scalar sector is of the first order and relates the cosmologically needed ΔB with the Higgs boson mass, requiring the Higgs boson mass less than 70 GeV (even in a more generous supersymmetric case) [23], which is already ruled out by the discovery of the Higgs boson at 125 GeV. Even if the phase transition were made to be of the first order, the CP violation induced by δ_{CKM} is known to be insufficient to generate an enough chiral asymmetries [24]. But, a caveat with two Higgs doublets has been discussed recently [25].

8.1.3. Affleck–Dine baryogenesis

There is also another mechanism where an evolving scalar(s) generates the baryon number. Irrespective of two or more decay channels commented in the GUT baryogenesis, if X in one-phase decays to another phase having a different baryon number then the baryon number in the final phase can be different from that in the initial phase, which has led to the Affleck–Dine (AD) mechanism [26]. The AD baryogenesis uses the baryon number carrying scalars in supersymmetric (SUSY) models. Quarks accompany their superpartners which are called squarks carrying the baryon number B . The vacua of scalars, including the squarks, can have different baryon numbers. The CP phases of complex scalars, such as those of squarks, can provide the effective CP violation. As the VEVs of scalars evolve, baryon number can be generated. It has been reviewed in Ref. [27].

This mechanism has been extensively studied for the flat directions in supersymmetric models [28]. Since the flat directions are also used extensively in the ADM scenario, we will discuss more on the AD mechanism in SUSY models in Section 8.3.2.

8.2. Creation of global quantum numbers

In the SM, the rank of the gauge group $\text{SU}(3) \times \text{SU}(2) \times \text{U}(1)$ is 4, and hence the baryon and lepton numbers, B and L , must be global quantum numbers. The simplest GUT $\text{SU}(5)$ has rank 4 and the vacuum of scalar fields preserve $B - L$. In addition, the interactions in the $\text{SU}(5)$ GUT, which has rank 4, preserve $B - L$. If B creation were made in the $\text{SU}(5)$ GUT phase above the EW scale, the $B - L$ quantum number must have been 0 even if B were made nonzero. On the other hand, the EW sphaleron processes preserve $B - L$ as shown in Fig. 8.1. The $B - L$ quantum number above the EW scale is preserved during the EW phase transition, and hence the $B - L$ quantum number generated in the $\text{SU}(5)$ GUT is zero below the EW scale. The individual B and L numbers below the EW scale is proportional

Table 8.1. Two channels for the N decay.

Majorana N		Final state	BR	L in final state
N	$\rightarrow$	$f_1 s_2$	r	L_1
N	$\rightarrow$	$\bar{f}_3 s_4$	$1 - r$	L_2
N^c	$\rightarrow$	$\bar{f}_1 \bar{s}_2$	$\bar{r}$	$-L_1$
N^c	$\rightarrow$	$f_3 \bar{s}_4$	$1 - \bar{r}$	$-L_2$

to $B - L$ if the sphaleron process is 100% effective [29]. Thus, the SU(5) GUT is not promising to generate B , considering the EW phase transition.

Thus, we need B and/or L generation, violating $B - L$, such that a nonzero $B - L$ is generated above the EW scale. In fact, the required $(B - L)$ -violating interaction is present in the SO(10) GUT because the rank of SO(10) is 5 and $B - L$ can be a gauged interaction.

Therefore, successful baryo- or leptogenesis can be realized in the SO(10) GUT. One can present baryogenesis in non-GUT examples as in the original leptogenesis example with heavy Majorana neutrinos [17], where the process $\Delta(B - L) = -\Delta L$ is constructed by the mass terms of heavy Majorana neutrinos. Generation of ΔB by $B - L$ violating interactions by heavy quarks was also suggested as “Q genesis” [18]. Since masses of the SM neutrinos can be related to the heavy Majorana neutrino masses, here we focus on the leptogenesis idea.

To create global charges, the so-called Nanopoulos–Weinberg theorem should be satisfied. The theorem requires two or more decaying channels of the mother particle [30, 31]. As an example, let us consider the leptogenesis, where a heavy Majorana neutrino N ($= N^c$) decays to two final states as shown in Table 8.1. The global charge that we consider in this example is the *lepton number* L . The final state lepton numbers are $L_{1,2}$ with branching ratios r and $1 - r$ (for antiparticles $\bar{r}$ and $1 - \bar{r}$ instead), respectively. Thus, from N and N^c decays, we obtain the lepton number $\Delta L = rL_1 + (1 - r)L_2 - \bar{r}L_1 - (1 - \bar{r})L_2$,

$$\Delta L = (r - \bar{r})(L_1 - L_2). \quad (8.2)$$

For a nonvanishing lepton number generation, therefore, both factors in Eq. (8.2) must survive. The factor $(L_1 - L_2)$ requires two different channels of N decay with different lepton numbers. A nonvanishing $(r - \bar{r})$ is provided by C and CP violations in the theory. Even though the CPT theorem dictates the same total decay rate (i.e., the inverse of lifetime) for N and N^c , the partial decay rates can be different for N and N^c decays if CP violation is present. These must be built in the theory to create a nonvanishing lepton number. The CP violation does not enter in the tree processes of Table 8.1. The CP violation is always an interference phenomenon as emphasized in Section 4.7. Thus, we must consider the interference terms between the tree and loop diagrams.

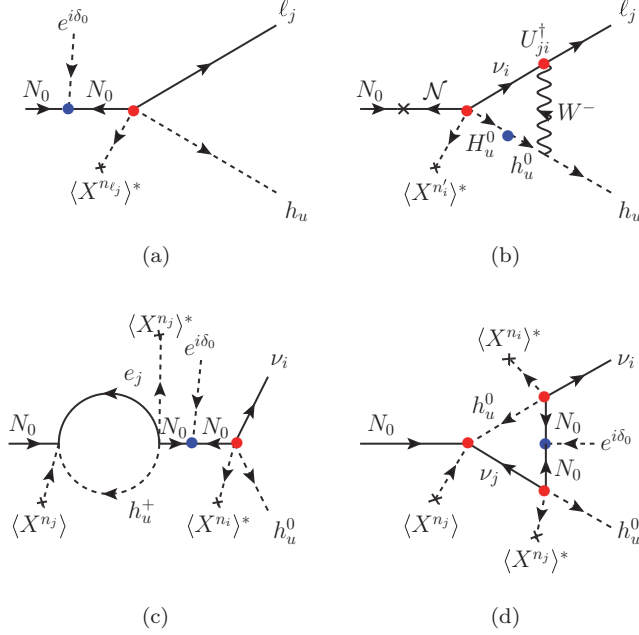


Fig. 8.3. The diagrams for leptogenesis: (a) the tree diagram, (b) the W exchange diagram in the Type-II leptogenesis, (c) the wave function renormalization diagram with the intermediate heavy neutrino in the Type-I leptogenesis, and (d) the vertex diagram in the Type-I leptogenesis. In each case, the final state leptons can be both ℓ_i and ν_i .

It is well known that heavy Majorana neutrinos in the loop generate the lepton number as shown in [32–34]. Here, we call it “Type-I leptogenesis”. In the Type-I leptogenesis, both the CP violation and the lepton number violation are inserted in the blue bullet in the heavy Majorana neutrino line in Figs. 8.3(a), 8.3(c) and 8.3(d). If we consider only one heavy lepton, i.e., N_0 , in the Type-I leptogenesis, there is no CP phase contribution since (a), (c) and (d) in Fig. 8.3 have the same phase. Thus, we must consider at least two heavy leptons as emphasized in Ref. [35]. Thus, the asymmetry has a suppression factor m_{N_0}/m_{N_j} where N_j is the additional heavy neutrino.

If the W -boson loop of Fig. 8.3(b) contributes, then it is called the “Type-II leptogenesis” [36]. For the Type-II leptogenesis to be appreciable, the EW symmetry must be broken. It requires that the EW symmetry is not restored at high temperature above the EW scale [37].³ With the W -boson contribution, the CP phase is inserted by the PMNS one at the W coupling vertex and the lepton number violation is given by inert scalar doublets (not participating in the EW symmetry breaking), i.e., H_u in Fig. 8.3(b) [36]. Also, one needs another neutral lepton $\mathcal{N}$. Then, in Type-II leptogenesis it is possible to relate the lepton asymmetry ϵ_L to

³In SUSY models, it is natural to break the EW symmetry above the EW scale [36].

the PMNS phase δ_{PMNS} of the SM. By converting L to B by sphaleron processes, the baryon asymmetry can be related to the phase δ_{PMNS} .⁴

8.3. Asymmetric dark matter

The DM scenario based on the asymmetric dark matter (ADM) is following the method of Section 8.2, employing a quantum number D from a global symmetry. This symmetry is called “DM global symmetry”, $U(1)_D$. Even though a DM particle may belong to the visible sector, the ADM scenario defines a sector possessing a DM particle as a separate one. In addition, the ADM mechanism is designed as follows [39]:

- (1) In both the visible and/or dark sectors, asymmetries are created, along the standard methods of baryogenesis or leptogenesis. Communication of the quantum numbers between the visible and dark sectors are possible. Or, baryon and DM asymmetries may be generated simultaneously.
- (2) Later, the process which communicates the asymmetry between the visible and dark sectors decouples, separately freezing in the asymmetry in the visible and dark sectors.
- (3) After the dark sector was thermalized having achieved the asymmetry generation, the symmetric part in the abundance must efficiently annihilate away.

If item (3) is not invoked, then the DM density is determined by the decoupling temperature as shown in Fig. 2.4 of Chapter 2. There are many ways to create the above cosmological history in particle physics models. But, most of these ways belong to the classes of *asymmetry transfer* and *asymmetry generation* as discussed for the generation of global charges in Section 8.2. The generation mechanism follows the lines of baryogenesis. The transfer mechanism uses the process similar to the sphaleron process, or the processes mimicking it. This set up for generation of DM is called ADM paradigm [40]. Since it has been extensively reviewed in [29, 41], here we focus only on a few scenarios which can be easily explained without much complication in terms of the theory we already discussed in Section 8.2.

The transfer mechanism can be used in both ways: first create the visible sector number (B and/or L) and transfer it to the DM number D , and second create the dark number D and transfer it to B and/or L . The resulting numbers of B and D are required to satisfy their cosmological abundances.

The asymmetry generation mechanism frequently accompanies the generation of B and L , in which case it is called *cogenesis*. On the other hand, if the DM generation has distinct mechanisms for generating the D asymmetry, it is called *darkogenesis*.

⁴There also exists an example relating δ_{PMNS} and δ_{CKM} [38].

Since the ADM mechanism uses a DM particle X and its antiparticle $\bar{X}$, the prediction depends on how efficiently X and $\bar{X}$ are annihilated. If their annihilation were not efficient, then the calculation of the DM abundance is similar to that of the WIMP abundance discussion of Chapter 7. If their annihilation were complete, then the calculation of the DM abundance is similar to that of the B abundance.

8.3.1. Renormalizable interactions

Because the global quantum number is considered in the ADM scenarios, the dark global symmetry $U(1)_D$ may not be exact with gravity consideration, viz. Section 6.6. In particular, we consider the global symmetry breaking $U(1)_D$ - $SU(2)_W$ - $SU(2)_W$ anomaly during the EW phase transition,

$$\partial_\mu j_D^\mu = \frac{Ng^2}{32\pi^2} W_{\mu\nu}^i \tilde{W}^{i\mu\nu}, \quad (8.3)$$

where j_D^μ is the current for the $U(1)_D$ symmetry, and N is the number of chiral $SU(2)_W$ doublets (the difference of the numbers of left-handed and right-handed doublets).

Most ADM scenarios prefer to satisfy the coincidence problem by asserting a light DM particle with mass around 1–10 GeV. A naive speculation for $\Omega_D/\Omega_{B-L} \approx m_X/m_p$ has been proposed by a mass ratio scenario that the DM particle is about five times heavier than proton because $\rho_{\text{CDM}}/\rho_B \approx 5$. Then, Z -boson can decay to X and $\bar{X}$. The DM may also scatter (through the Z -boson exchange) in the direct DM detection experiments (with cross section in the range of 10^{-39} cm^2). These practically rule out the (natural scale) renormalizable interactions between the DM and $SU(2)_W$ doublets. However, note that one can consider some suppression factors with respect to the natural scale, to fine-tune at the observed level [42]. In Fig. 8.4 (Fig. 1 of Ref. [43]), the fine-tuning conditions between the DM mass and the decoupling temperature are shown.

8.3.2. Nonrenormalizable interactions

Thus, nonrenormalizable interactions have been considered, which is shown schematically in Fig. 8.5 in terms of $\mathcal{O}_{B-L}$ and $\mathcal{O}_X$. For example, in the visible sector the following nonrenormalizable operators, carrying nonvanishing $B-L$, can be considered

$$\Omega_{B-L} = u^c d^c d^c, q \ell d^c, \ell h_u, \quad (8.4)$$

where u^c, d^c, e^c are right-handed antiquarks and charged leptons, q and ℓ are left-handed quark and lepton doublets, and h_u is the up-type Higgs doublet. For $\mathcal{O}_X$, the simplest combination of DM fields X , carrying n units of D , can be considered

$$\Omega_X = X^n. \quad (8.5)$$

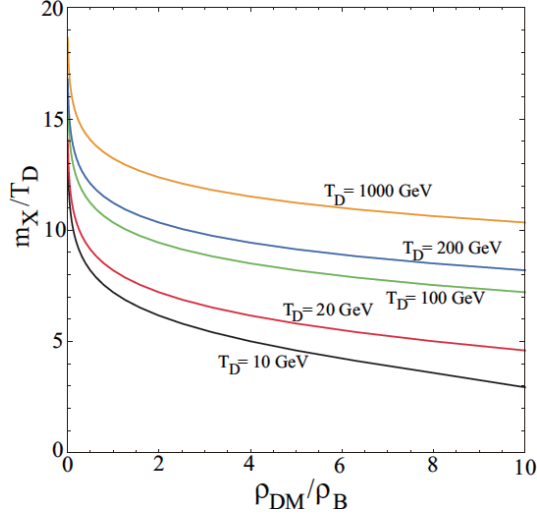


Fig. 8.4. The ratio of ADM energy density ρ_{DM} to baryon density ρ_B as a function of DM mass m_X in units of temperature at which the $B-X$ transfer decouples at T_D , for labeled values of T_D .

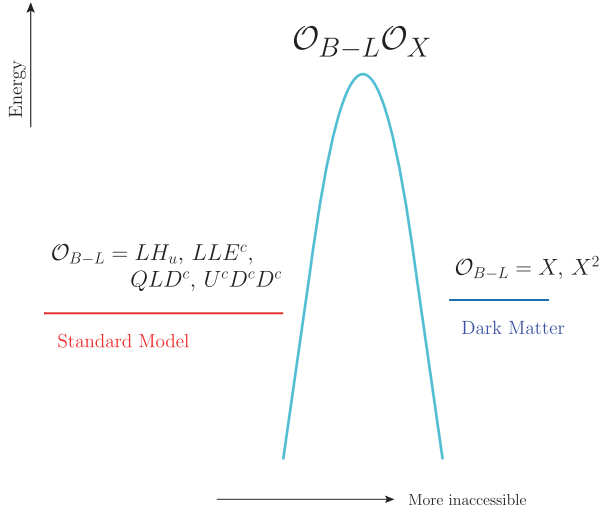


Fig. 8.5. A schematic view of higher dimensional ADM models [44].

We will briefly comment on the flat directions in the SUSY AD mechanism for generating B , and its application to the ADM scenario via Fig. 8.5.

Flat directions in the SUSY AD mechanism of B generation

The seed for an effective B generation in the SUSY AD scenario is during and right after inflation, where the inflaton energy acts as vacuum energy. In this case, a

flat direction of (8.4) can easily have a minimum far from the origin, giving rise to large expectation values for squark and/or slepton fields. Here, we sketch the idea presented in [28]. The effective mass of the flat direction of ϕ ($\equiv$ AD field) during this epoch is very large

$$m_{\phi,I} \simeq H, \quad (8.6)$$

For example, a D -term in SUSY is

$$\delta K = \int d^4\vartheta \frac{1}{M_{\text{P}}^2} \chi^\dagger \chi \phi^\dagger \phi, \quad (8.7)$$

where χ is a field which dominates the energy density of the Universe, ϕ is a canonically normalized flat direction. δK can generate an effective mass term for ϕ , $\mathcal{L} = (\rho/M_{\text{P}}^2) \phi^\dagger \phi$, i.e., (8.6) with $\rho = 3H^2 M_{\text{P}}^2$. But the final baryon number is given when everything is settled down with a gravitino scale m_ϕ ,

$$\frac{n_B}{s} \approx \frac{n_B}{n_\phi} \frac{T_R}{m_\phi} \frac{\rho_\phi}{\rho_I}, \quad (8.8)$$

where n_B and n_ϕ are baryon and AD field number densities, T_R is the reheat temperature, $m_\phi \sim m_{3/2}$ is the low energy mass for the AD field, and ρ_ϕ and ρ_I are the AD field and inflaton mass densities (both at the time of inflaton decay).

The curvature of the potential is of the order of the (instantaneous) Hubble constant. Thus, if the minimum of the potential is at the origin as in the minimal Kähler potential, quantum fluctuations of ϕ during inflation will not lead to a net baryon number since the correlation volume for the fluctuations is generally much smaller than the present Hubble volume. So, this AD scenario needs models with the minimum of the potential of ϕ far from the origin. Nonminimal Kähler potentials can allow this possibility [28]. Note that in this regard, if there is a point of enhanced symmetry on the moduli space, the potential (no matter what the source) is necessarily an extremum about this point (for the potential induced by the finite density breaking this follows since the Kähler potential is a minimum about a symmetry point). For example, with the SM fields, the origin is always an enhanced symmetry point, and the potential is always an extremum at the origin.

Unlike the case of renormalizable interactions, the effective potential from non-renormalizable interactions can induce a mass for a flat direction which is roughly independent of the magnitude of the AD field. For large fields, therefore, nonrenormalizable interactions are more important than renormalizable ones. Reference [28] made a further assumption that after inflation, the Universe enters into a matter-dominated epoch where the energy is carried by coherent oscillations of the inflaton as discussed in Chapter 6. For the AD mechanism, assuming the initial baryon number averages to zero over the current horizon size, only the zero mode of the field is relevant. The evolution of the AD field parameterizing a flat direction is governed as usual by the classical equations of motion, that of a damped oscillator.

For the global charge generation out of nothing, we also satisfy Sakharov's second condition on the existence of "C and CP violation". For C violation, we refer to Fig. 2.8. In the SUSY AD scenario, usually the coefficient of the A -term is in general complex. Also, the ϑ^0 components of the AD superfields are complex. The relative phase between the A -term and the "initial" phase of the flat direction is the source of CP violation in the SUSY AD mechanism. The nonzero number density of this phase field is obtained if it changes in time, otherwise the Δn_ϕ is not obtained. At early times the potential for the phase of ϕ goes like $\cos(\theta_a + \theta_\lambda + n\theta)$, where λ is a parameter in the superpotential and a is an $O(1)$ parameter during inflation. Let θ_A be the phase of the SUSY breaking A -term at the $m_{3/2}$ scale. As the Hubble parameter H decreases below $m_{3/2}$ the low energy A -term becomes more important and the angular potential goes like $\cos(\theta_A + \theta_\lambda + n\theta)$. When the field begins to oscillate freely, a nonzero $\dot{\theta}$ is therefore generated if $\theta_a \neq \theta_A$. This is of course required in order to generate a nonzero baryon number since $n_B = 2|\phi|^2\dot{\theta}$. The resulting baryon number therefore depends on the CP violating phase $\theta_a - \theta_A$, i.e., on a relative phase between the inflaton (θ_a) and the SUSY breaking (θ_A) sectors.

For baryogenesis, it is important to know the sign of mass squared near $\phi = 0$. As discussed above, with minimal Kähler potential terms, m^2 is of order H^2 with positive coefficient. In this case, the AD baryogenesis does not work because ϕ settles to 0 quickly. However, if the sign of the induced mass squared is negative, a large expectation value for a flat direction can develop. With nonminimal Kähler terms, it has been argued [28] that this is as plausible as a positive mass squared. The magnitude of the field is then set by a balance with nonrenormalizable terms in the superpotential which lift the flat direction. To get an idea how Ref. [28] has solved the evolution problem numerically, we present their equations of motion for the real and imaginary parts

$$\begin{aligned}
\ddot{\phi}_R + \frac{2}{t}\dot{\phi}_R + \left(m_\phi^2 - \frac{c'}{t^2}\right)\phi_R + A|\phi|^{n-1}\cos((n-1)\theta) \\
+ (n-1)|\phi|^{2n-4}\phi_R = 0, \\
\ddot{\phi}_I + \frac{2}{t}\dot{\phi}_I + \left(m_\phi^2 - \frac{c'}{t^2}\right)\phi_I - A|\phi|^{n-1}\sin((n-1)\theta) \\
+ (n-1)|\phi|^{2n-4}\phi_I = 0,
\end{aligned} \tag{8.9}$$

where $\phi = \phi_R + i\phi_I$, and $\theta = \arg. \phi$.

The SUSY ADM with the AD mechanism

In the SUSY AD scenario, following the B generation discussed above, we use the nonrenormalizable interactions of the form

$$W = \frac{\mathcal{O}_D \mathcal{O}_{B-L}}{M^{m+n-3}}, \tag{8.10}$$

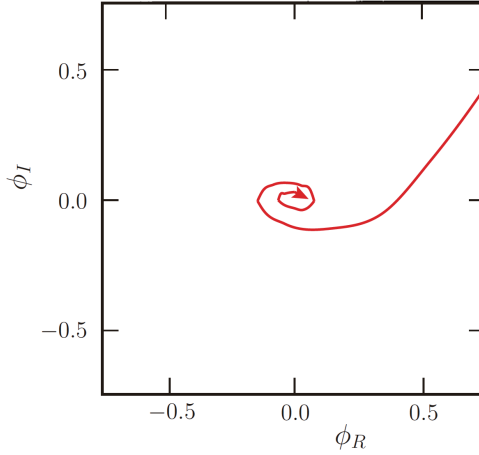


Fig. 8.6. The spiraling curve from [28]. It is a numerical solution of Eq. (8.9) for $n\theta_i = \frac{9}{10}\pi$ with $m_\phi = c' = -A = 1$, and $n = 4$.

where m is the dimension of $\mathcal{O}_{B-L}$. The lowest dimensional operators in the SUSY AD scenario take the form

$$W = \frac{Xu^c d^c d^c}{M}, \frac{Xql d^c}{M}, \frac{Xlle^c}{M}, \quad (8.11)$$

which have flat directions in $D-B$, $D+L$, and $D+L$, respectively. The above higher dimension operators in Eq. (8.11) can be implemented in principle in GUTs [45] or in string compactification [46]. An operator similar to LHX^2 was also implemented in [47]. The symmetries mentioned above has an exact $D+B-L$ symmetry. Sphaleron processes described in Fig. 8.5 convert $B-L$ to D , and vice versa, i.e., the “transfer mechanism”. When the interactions decouple, $B-L$ and D symmetries each are separately restored, freezing in the $B-L$ and D numbers separately. This is a conversion mechanism. Also, as in the EW baryogenesis case, cogenesis of D and $B-L$ can be achieved with the corresponding sphaleron of Fig. 8.6.

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Chapter 9

Detection

*All truths are easy to understand once they are discovered;
the point is to discover them — Galileo Galilei*

9.1. Introduction

The evidence that the Universe contains about 27% cold dark matter (CDM) of Fig. 1.2 is solely based on the cosmological observation, which needs to be proved by another independent method. The CDM property in the cosmological observation is based on the *cold* matter property when the Universe went through the radiation–matter equality period.

The expected additional proofs are classified broadly into three categories. If the source of CDM is a very light boson such as the bosonic collective motion (BCM) [1], one can consider firstly its (long range force) effect detectable in the Cavendish-type experiments and second probing creation of SM particles via its interactions. Third, if the source of CDM is due to stable or almost stable particle such as WIMP (requiring $\tau \gtrsim 10^{26}$ yrs, much longer than the Universe age t_U), the effect may be detectable by producing them in high energy accelerators or its scattering with SM particles or by its annihilation in the cosmos to SM particles [2]. In this chapter, we review briefly the efforts to detect CDM particles by these three methods.

9.1.1. *Bosons or fermions?*

At present, it is not known what is the spin of CDM particle. Of course, if CDM is BCM, then its spin is zero. If CDM is a kind of massive particle, its spin can be 0, $\frac{1}{2}$, 1, or $\frac{3}{2}$. The spin $\frac{3}{2}$ case is the gravitino DM, which has been studied extensively in Ref. [3]. At present, we do not have a clue on the spin.

The most widely studied case is spin $\frac{1}{2}$ WIMP, and in this chapter also, we will pay much attention on the spin $\frac{1}{2}$ case.

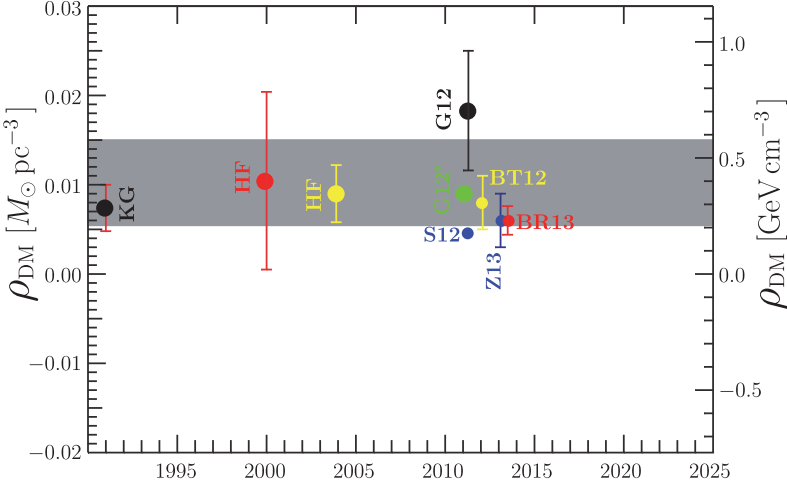


Fig. 9.1. The local DM density [4].

9.1.2. Local DM density

Detection possibility of cosmic dark matter (DM) depends on its local density, i.e., at the Earth position based on the density distribution assumption in the Milky Way. We used the local density of DM of $(0.3\text{--}0.45)\text{ GeV cm}^{-3}$ before [3]. The recent observations, however, allows a wider range [4],

$$(0.2\text{--}0.6)\text{ GeV cm}^{-3}. \quad (9.1)$$

The DM density is calculated locally by the vertical kinematics of stars near Sun — called tracers [11], which is denoted as ρ_{dm} . The global estimate of local density is by extrapolating the rotation curve at a far halo to Sun's position, which is denoted as $\rho_{\text{dm,extr}}$. A naive guess is to equate them. But there are possibilities of $\rho_{\text{dm}} < \rho_{\text{dm,extr}}$ or $\rho_{\text{dm}} > \rho_{\text{dm,extr}}$. Some physical implications of these possibilities are discussed in [4].

In Fig. 9.1, we present Fig. 2 of Ref. [4], which lists the estimates of ρ_{dm} of Refs. [5–12]. These plots use the baryon density $\rho_b = 0.0914 M_{\odot} \text{ pc}^{-3}$ and the surface density $\Sigma_b = (55 \pm 4.9) M_{\odot} \text{ pc}^{-2}$ [13]. The green point is from [8] by a stronger prior on $\Sigma_b = (55 \pm 1) M_{\odot} \text{ pc}^{-2}$.

9.2. Detection of nongravitational long range forces

With the discovery of Higgs boson, it is now known that a fundamental spin-0 particle exists. It is a strong hint that more spin-0 particles exist in nature. These include very light scalars and very light pseudoscalars. Also, the possibility of very light spin-1 particles mixing with the SM photon has been considered [14], which became recently popular with the name *dark photon* [15] because of the possibilities

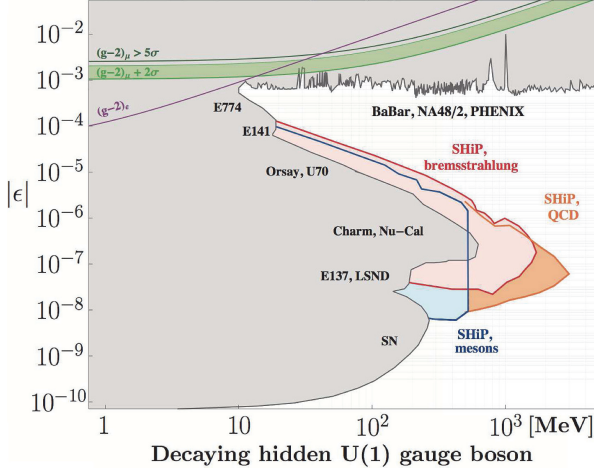


Fig. 9.2. Experimental constraints on the parameters α (coupling strength) and λ (range) [20].

of $U(1)'$ gauge bosons acting on DM to account for a possible additional neutrino number in view of the Planck data [16]. These possibilities are extensively reviewed in [17].

9.2.1. Dark photon

The dark photon, a hypothetical elementary particle acting on DM, can act as dark radiation energy (in the sense that it cannot be observed as luminously as photon) if its mass is sufficiently small, i.e., less than 1 MeV, during the nucleosynthesis epoch. Then, its energy density can be counted as the neutrino energy and hence contributes to some effective neutrino number. It can theoretically mix with ordinary photons via interactions of BSM particles interacting with both DM and SM particles. Its effects, however, cannot be completely hidden outside the moment of the nucleosynthesis era. It is because of its mixing possibility with the SM photon.

The mixing parameter ϵ denotes the γ and $U(1)'_{\text{dark}}$ -gauge-boson mixing, $\frac{1}{2}\epsilon F_{\mu\nu}F'_{\mu\nu}$ [14]. $A'_{\mu \text{ dark}}$ can be massless or unstable. Unstable spin-1 particles under this category is also called dark photon. So, particles charged under $U(1)'_{\text{dark}}$ gauge group interacts much more weakly than ordinary charged particles and thus are called *milli-charged particles*. The laboratory and cosmological bound of milli-charged particles was studied sometime ago [18], excluding mixing parameters of the order of fine structure constant as shown in Fig. 9.2. Theories of grand unification and beyond, however, allows only ϵ at the grand unification coupling strength, typically at the order of fine structure constant. If the dark photon decays, then there are numerous ways to probe its decay products, which constrain its coupling constants with matter. Figure 9.2 summarizes these bounds from various experiments and shows possibilities of the future sensitivity.

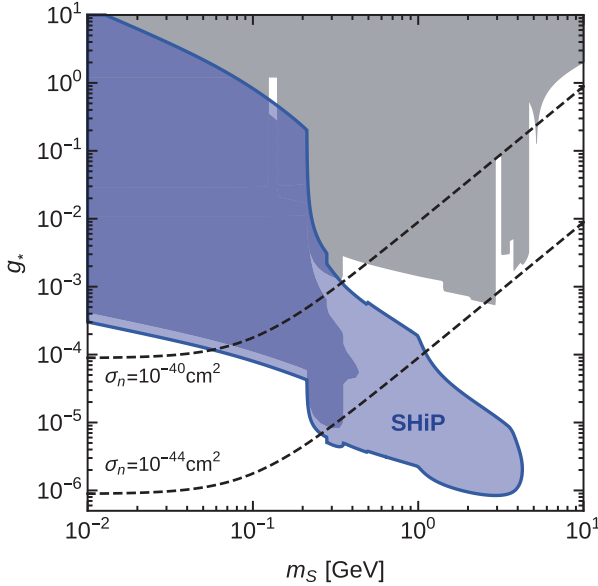


Fig. 9.3. Projected sensitivity for Yukawa-like couplings of S [17].

For a light scalar particle, Ref. [17] also shows the bounds on the strength of Yukawa couplings as shown in Fig. 9.3.

9.2.2. The Cavendish-type experiments

The Cavendish-type experiments are designed to measure Newton's gravitational constant very accurately. The deviations are parameterized for two masses M and m by the effective range λ and the coupling α ,

$$V_Y(r) = -G_\infty \frac{Mm}{r} (1 + \alpha e^{-r/\lambda}). \quad (9.2)$$

With this simple form, the laboratory effort to bound the parameters α and λ has begun from [20], and the current bound is summarized in Fig. 9.4. Deviations from the inverse square law of gravity hint additional force carriers, most probably the existence extra U(1) gauge bosons. But, the possibility of an almost massless extra U(1) gauge boson is extremely difficult to be realized with a reasonable gauge coupling constant as shown at the lower left corner of Fig. 9.2.

On the other hand, very light scalars and pseudoscalars can affect the inverse square law, most effectively on nucleons which have spins. The effective potential mediated by these spin-0 bosons can be distinguished by the boson vertex to the nuclear spin: monopole-type and dipole-type. The scalar vertex is of monopole type, and the pseudoscalar vertex is called dipole type for which the Feynman diagrams are shown in Fig. 9.5 [19]. So, the long range interactions with scalar-scalar or

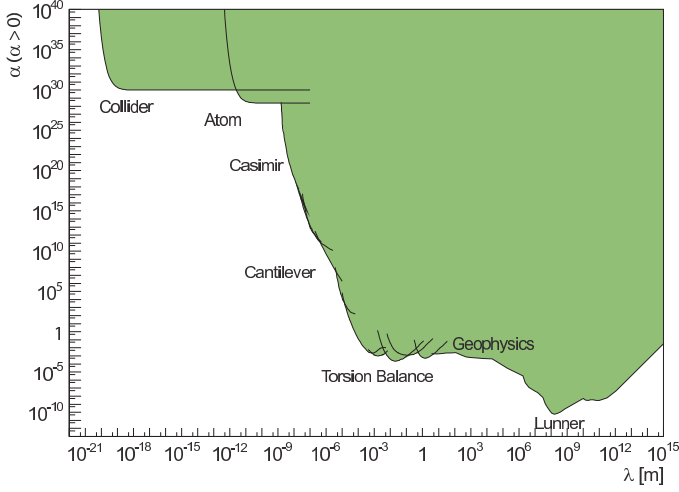


Fig. 9.4. Experimental constraints on the parameters α (coupling strength) and λ (range) [21].

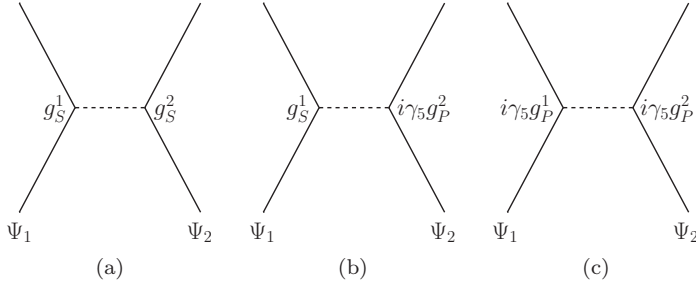


Fig. 9.5. Feynman diagrams for g_S and $i\gamma_5 g_P$ couplings.

pseudoscalar–pseudoscalar couplings are parity conserving and have a general form given in Eq. (9.2). The scalar–pseudoscalar couplings at two vertices have the following long range force form [19]:

$$V_Y(r) = g_S^1 g_P^2 \frac{\vec{\sigma}_2 \cdot \hat{r}}{8\pi M_2} \left(\frac{m_\varphi}{r} + \frac{1}{r^2} \right) e^{-rm_\varphi}, \quad (9.3)$$

where φ is the mediating spin-0 particle and M_2 is the nucleus mass having the pseudoscalar coupling, as shown in Fig. 9.5(b). For the preferred values of g_S and g_P , one can check whether the long range force limits of Fig. 9.2 exclude the considered region or not. Comparing the $1/r$ terms in (9.3) and (9.2), the light mass m_φ appears in the numerator of (9.3). So, it is expected that it is very difficult task to probe light pseudoscalars by the Cavendish-type experiments.

9.3. Detection of light pseudoscalars

The axion couplings come in three types: the PQ symmetry preserving derivative coupling c_1 term, the PQ symmetry breaking c_2 term, and also the PQ symmetry breaking anomalous c_3 term as discussed in Chapter 6. For the coupling of axion and the gluon anomaly to be present, $c_2 + c_3$ must be nonzero. Generally, discarding the fine-tuning of the couplings between the singlet σ and the BEH doublets, i.e., setting $c_2 = 0$, the “invisible” axion coupling to gluons is given by

$$\frac{a}{f_a} \frac{1}{32\pi^2} G_{\mu\nu}^a \tilde{G}^{a\mu\nu}. \quad (9.4)$$

Then, we note that this kind of nonrenormalizable anomalous term can arise in several ways. The natural scales of f_a are shown in Tables 6.1–6.3 of Chapter 6. The essence of the axion solution is that the axion VEV $\langle a \rangle$ seeks $\theta = 0$ now in our cosmos whatever happened before and solves the strong CP problem. So, the search efforts of the cosmic axions utilize the currently oscillating axion field even though its amplitude is extremely small, $|\langle a \rangle|_{\max} \simeq 10^{-19} f_a$. The solar axion search does not use this oscillating axion field, but tries to detect keV range photons created via solar axions by the Primakoff vertex [22].

The axion-like particles (ALPs) are defined to have their couplings to $SU(2)_W$ anomalies in the absence of coupling to the $SU(3)_c$ anomaly. Therefore, there exists the ALP–photon–photon coupling of the form

$$\frac{a_{\text{ALP}}}{f_{\text{ALP}}} \frac{1}{32\pi^2} F_{\text{em}\mu\nu} \tilde{F}_{\text{em}}^{\mu\nu}. \quad (9.5)$$

Unlike the QCD axion, a_{ALP} does not have a relation between the ALPs mass m_{ALP} and f_{ALP} , and they are treated independently.

9.3.1. Axion detection experiments

The axion detection experiments up to 2010 have been reviewed in Ref. [3]. Here, we sketch it and add more recent detection ideas.

Currently, there are a variety of experiments searching for axions. The core of these experiments use axions interacting with SM fields shown in Fig. 9.6, and they rely on the Primakoff process for which the following coupling, $c_{a\gamma\gamma}$ is given in Eqs. (9.4) and (9.5):

$$\mathcal{L} = c_{a\gamma\gamma} \frac{a}{f_a} \{F_{\text{em}} \tilde{F}_{\text{em}}\}, \quad c_{a\gamma\gamma} \simeq \bar{c}_{a\gamma\gamma} - 2.0, \quad \text{for } \frac{m_u}{m_d} \simeq 0.5, \quad (9.6)$$

where $c_{a\gamma\gamma}$ are tabulated in Tables 6.1–6.3 of Chapter 6. The curly bracket $\{ \}$ implies the inclusion of $1/32\pi^2$.

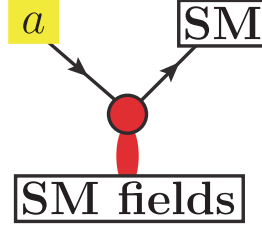


Fig. 9.6. Axion detection process. The SM fields can be a static magnetic field $\mathbf{B}$ or oscillating electric dipole moment. The interaction blob is the Primakoff interaction $a\mathbf{E}\cdot\mathbf{B}$ where $\mathbf{E}$ is oscillating, following the cosmic oscillation of $\langle a \rangle$ in the case of haloscope or an axion quantum in the case of helioscope. The detected field shown as SM is electromagnetic wave converted to an electric current.

9.3.2. Laser searches

There is a class of laboratory axion searches which utilize laser photons (γ_{laser}) traversing a magnetic field in contrast to detection schemes on axions coming from the sky. Here, the polarized laser photons can scatter off the laboratory magnetic field (considered to be virtual photons (γ_v)) and convert into axions $\gamma_{\text{laser}} + \gamma_v \rightarrow a$. Currently, laser axion searches have fallen into two general categories. The first technique looks for magneto-optical effects of the vacuum due to polarized laser photons disappearing from the beam as they are converted into axions. The second looks for photons converting into axions in the presence of a magnetic field, which are then transmitted through a wall and converted back into photons by a magnetic field on the other side, the so-called “light shining through walls” experiments.

Polarization shift of laser beams

The axion–photon–photon anomalous coupling of Eq. (9.6) is the key interaction here. The axion-like particle search induced by laser beams has been performed since early 1990s by the Rochester–Brookhaven–Fermilab–Trieste (RBFT) group [23], and later the PVLAS collaboration has performed with an initial positive signal with $f_a \sim 10^6$ GeV [24] which went away eventually.

Here, the method is looking for polarization of the laser beam. With more data accumulation, there is no convincing evidence for an axion-like particle with $f_a \sim 10^6$ GeV at present, contrary to an earlier confusion [24–27]. This incident, however, has ultimately lead to the current search of ALPs II experiment on the light shining through walls at DESY [28].

Light shining through walls

The “light shining through walls” technique for searching for axions was first proposed in 1987 [29]. The general experimental layout is sketched in Fig. 9.7 where polarized laser photons pass through the magnetic field with $\mathbf{E} \parallel \mathbf{B}$ between mirrors

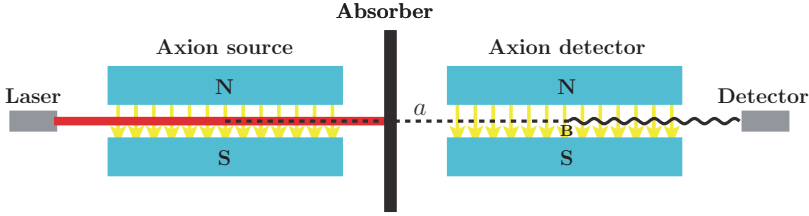


Fig. 9.7. A sketch of an experiment for the light shining through the wall.

and any converted axions (or other pseudoscalar particles) can continue through an absorber to be reconverted to photons due to the $\mathbf{B}$ field on the other side.

The probability for a photon to convert into an axion as it traverses the “Axion Source” region is given by

$$P_{\gamma \rightarrow a} \propto \frac{1}{4} \left(\frac{\alpha_{\text{em}} c_{a\gamma\gamma}}{2\pi F_a} BL \right)^2 \frac{1 - \cos(qL)}{(qL)^2}. \quad (9.7)$$

This is the same probability for an axion to convert back into a detectable photon in the “Axion Detector” region on the other side of an absorber, which leaves the total probability for detecting a photon–axion–photon conversion as $P_{\gamma \rightarrow a \rightarrow \gamma} = P_{\gamma \rightarrow a}^2$ (ignoring photon detection efficiencies of course) [30]. There is a maximum detectable axion mass for these laser experiments as a result of the oscillation length becoming shorter than the magnetic field length causing a degradation of the form factor $F(q) = 1 - \cos(qL)/(qL)^2$ but this can be compensated for by multiple discrete dipoles.

Recently, it has been shown that photon regeneration experiments can be resonantly enhanced by encompassing both the production and reconversion magnets in matched Fabry–Perot optical resonators [31].

Magneto-optical Vacuum Effects

An alternative to the “shining light through walls” technique is to look for the indirect effect of photons in polarized laser light converting into axions as the beam traverses a magnetic field. The initial experiment for magneto-optical vacuum effects were carried out by the RBFT Collaboration [32].

Figure 9.8 illustrates the two different ways in which axion interactions can modify a polarized laser beam: (a) induced dichroism and (b) vacuum birefringence. Vacuum dichroism occurs when a polarized laser beam passes through a dipole magnet with the electric field component $\mathbf{E}$ at a nonzero angle ϕ relative to the $\mathbf{B}$. The photon component parallel to the $\mathbf{B}$ will have a small probability to convert into axions causing the polarization vector to rotate by an angle ϵ .

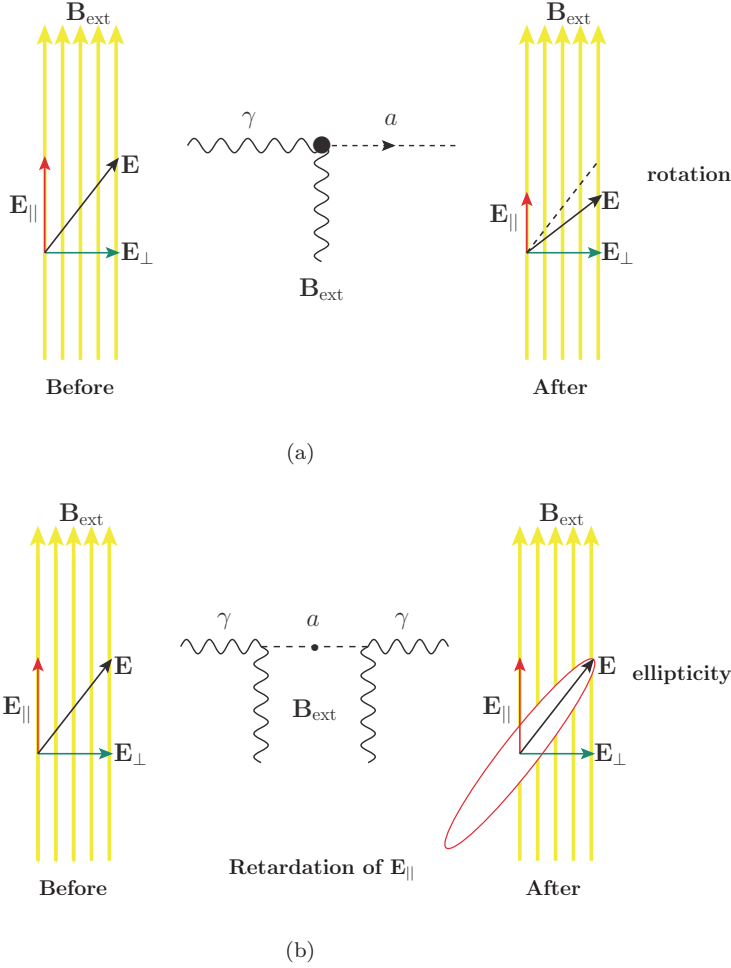


Fig. 9.8. (a) The dichroism: photons converting to axions cause a rotation of a linearly polarized laser beam. (b) The birefringence: the ellipticity is induced by virtual axions.

The early PVLAS collaboration reported the positive detection of vacuum dichroism. This experiment consists of a 1 m long 5 T superconducting magnet with an angular frequency Ω_{mag} of the magnet rotation and a 6.4 m long Fabry–Perot cavity giving the pass number $N = 2\Omega_{\text{mag}}/\pi \sim 44,000$. Here, N is the number of paths the light travels in the magnetic field. ϵ is estimated as

$$\epsilon \approx N \frac{B^2 L^2}{64} \left(\frac{c_a \gamma \gamma}{f_a} \right)^2 \sin(2\theta), \quad (9.8)$$

in the limit that $m_a^2 L/4\omega \ll 1$ where L is the effective path lengths. It registered a polarization shift of

$$\epsilon = (3.9 \pm 0.5) \times 10^{-12} \text{ rad pass}^{-1}, \quad (9.9)$$

which translates to an allowed mass range of a neutral pseudoscalar boson of $1 \text{ meV} \leq m_b \leq 1.5 \text{ meV}$ and a coupling strength of $1.5 \times 10^{-3} \text{ GeV}^{-1} \leq c_{a\gamma\gamma}/f_a \leq 8.6 \times 10^{-3} \text{ GeV}^{-1}$ [24]. Though the report of this positive signal has been retracted, the interest it raised has lead to a number of more advanced experimental searches such as some of the new laser regeneration experiments mentioned previously.

Vacuum birefringence is due to the induced ellipticity of the beam (Ψ) as a result of virtual axions. It should be noted that higher order QED diagrams, or “light-by-light scattering” diagrams, are expected to contribute to vacuum birefringence as well. Each of these effects can be estimated as

$$\Psi \approx N \frac{B^2 L^3 m_a^2}{384\omega} \left(\frac{c_{a\gamma\gamma}}{f_a} \right)^2 \sin(2\theta), \quad (9.10)$$

in the limit that $m_a^2 L/4\omega \ll 1$, and ω is the photon energy and θ is the photon polarization relative to the magnetic field [30].

9.3.3. Solar axion search

Bragg diffraction scattering

Before discussing the search methods employing the cavity detectors, let us first comment on the solid-state crystal detectors mainly used for WIMP detection. Using the Bragg diffraction scattering, X-rays generated by coherent axion-to-photon conversion can be detected [33]. In this way, several WIMP CDM search collaborations were able to look through their data sets to constrain solar axion detection rates: germanium experiments COSME [34] and SOLAX [35], the reactor germanium experiment TEXONO [36], NaI crystal experiment [37]. These limits can be seen in Fig. 9.9.

Axion helioscopes

Axions produced in Sun’s nuclear core will free-stream out and can possibly be detected on Earth via an axion helioscope [38, 39]. The technique relies on solar axions converting into low energy X-rays as they pass through a strong magnetic field. A prototype detector was made in Tokyo [40], and a practical detector (possibly touching the KSVZ line) was designed in 1988 [41]. The flux of axions produced in the Sun is expected to follow a thermal distribution with a mean energy of $\langle E \rangle = 4.2 \text{ keV}$. The integrated flux at Earth is expected to be $\Phi_a = g_{10}^2 3.67 \times 10^{11} \text{ cm}^{-2} \text{ s}^{-1}$ with $g_{10} = (\alpha_{\text{em}}/2\pi f_a) c_{a\gamma\gamma} 10^{10} \text{ GeV}$. The probability

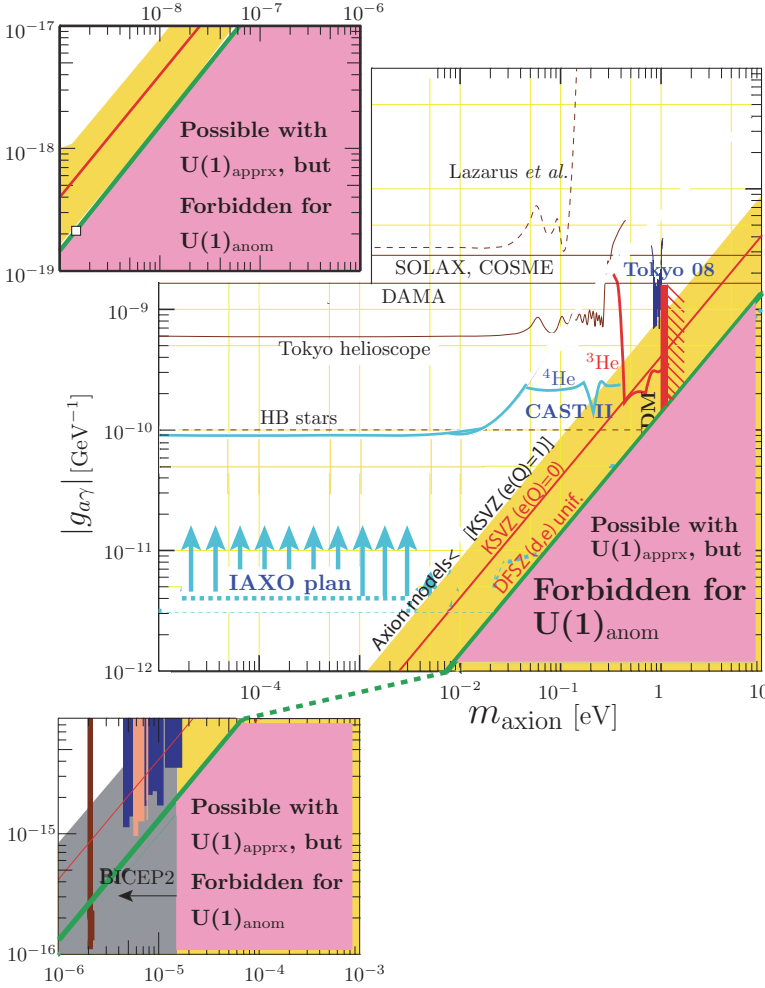


Fig. 9.9. The $g_{a\gamma}$ vs. m_{axion} in several model parameters. Axion detection experiments are also shown in the plan of Fig. 6.15.

of a solar axion converting into a photon as it passes through a magnet with field strength $\mathbf{B}$ and length $\mathbf{L}$ is given as

$$P = \left(\frac{\alpha_{\text{em}} c_{a\gamma\gamma} B L}{4\pi F_a} \right)^2 2L^2 \frac{1 - \cos(qL)}{(qL)^2}, \quad (9.11)$$

where q is the momentum difference between the axion and the photon, defined as $q = m_a^2/2E$ with the photon energy E . To maintain maximum conversion probability, the axion and photon fields need to remain in phase over the length of the magnet, thus requiring $qL < \pi$ [41]. For low mass axions $q \rightarrow 0$ leading to a maximum conversion probability. More massive axions will begin to move out of phase

with the photon waves though this can be compensated for by the addition of a buffer gas to the magnet volume, thus imparting an effective mass to the conversion photon [41] and bringing the conversion probability back to the maximum. Various axion masses can be tuned to by varying the gas pressure.

Using $B = 9$ Tesla magnet with $L = 9.3$ m, the first phase of the CERN Axion Solar Telescope (CAST) had run successfully since 2003, touching the KSVZ line [42, 43].

9.3.4. Search for cosmic axions

Finally, let us discuss the detection method of the cosmic axions with mass in the range 10^{-5} – 10^{-2} eV. Cosmic axions left over from the Big Bang may be detected utilizing microwave cavity haloscopes [38]. If the cavity is immersed in a solenoid, the exact treatment of current at the solenoid is impossible. So, just the resonance condition is used [39].

Solenoid enclosed in a cavity resonator — On the other hand, if the solenoid is immersed in the cavity of a tube design as shown in Fig. 9.10 [46], the explicit calculation of resonant modes is possible in the axion-electrodynamics [44, 45]. We can divide the volume of a tube into a region applied by a magnetic field and the rest free of the external magnetic field. Let us consider the tube of radius R_c . Then we apply an external magnetic field $B_0 = nI$ longitudinally over a region of a concentric cylinder of radius R_B ($R_B < R_c$), as shown in Fig. 9.10. If the coils in the solenoid are wound in a single thread entering from one end exiting at the other, there would be a net longitudinal current I which produces a static azimuthal magnetic field $((I/2\pi r)\hat{\theta})$ outside the solenoid, which can excite a TE mode. However, since this azimuthal field is much weaker than the longitudinal magnetic field $B_0 = nI$, the ratio is smaller than $1/2\pi nR_B$ which is practically negligible with a very large value of n . We can also make this azimuthal field even weaker by winding the coils in a way entering and exiting at the same end for cancellation of magnetic

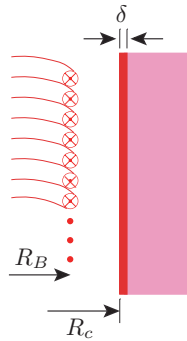


Fig. 9.10. The cylindrical cavity has radius R_c and length ℓ . The static external magnetic field $\mathbf{B}_0$ is applied longitudinally for the volume of radius $R_B \leq R_c$. The skin depth δ is shown for the cavity wall.

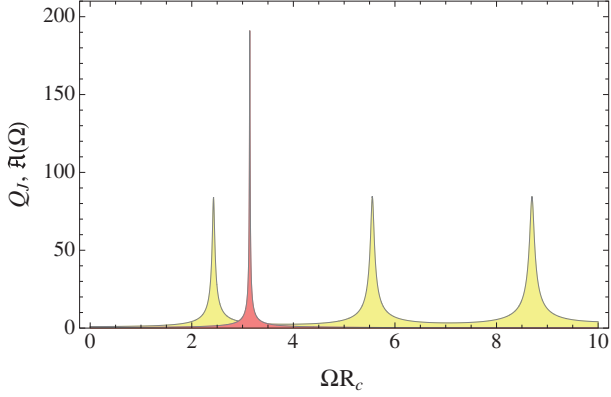


Fig. 9.11. An illustration of axion-tube resonance ($Q_l \sim 100$, $Q_a \sim 300$, $m_a \sim 1.3\omega_1$). The yellow curve is Q_J as a function of ωR_c and the reddish one is $|\mathcal{A}(\omega)|$ peaked at $m_a R_c$. A resonance occurs when the center of $|\mathcal{A}(\omega)|$ coincides with one of the peaks of Q_J , i.e., $\omega_l \simeq m_a$. The actual resonance curves would be much sharper.

fields. Since the static magnetic flux generated by the solenoid should not reenter the region exterior to the solenoid but interior to the tube, we make the solenoid much longer than the tube itself. Thus, this annular region is made free of the strong return flux.

For this setup, we can solve equations in each region and match the boundary conditions. The result is shown in Fig. 9.11. The maximum collection occurs at $\omega_l \simeq m_a$. Even if the solenoid is outside the cavity as in Ref. [38], still the resonance condition is valid.

Primordial CDM axions, drifting through the microwave cavity detectors, can resonantly convert to microwave photons, where their feeble interactions can be in part compensated by their large numbers; since the number density goes as $\sim f_a^2$ while their cross-section goes as $\sim 1/f_a^2$. If the axion makes up the majority of CDM in the Universe, its local density is expected to be roughly $0.3\text{--}0.45\text{ GeV/cm}^3$ [47], which yields a number density of $\sim 10^{14}$ axions/cm³ if one assumes a $4.5\text{ }\mu\text{eV}$ axion. The expected microwave signal will be a quasi-monochromatic line beginning at the microwave frequency corresponding to the axion mass and slightly broadened upward due to the axion virial distribution, with expected velocities of order $10^{-3}c$ implying a spread in energies of $\delta E/E \sim 10^{-6}$.

General detector properties

Since the Lagrangian for axions coupling to a magnetic field goes as

$$\mathcal{L}_{a\gamma\gamma} = \left(\frac{\alpha_{\text{em}} c_{a\gamma\gamma}}{2\pi f_a} \right) a \mathbf{E} \cdot \mathbf{B}, \quad (9.12)$$

the only resonant modes which can couple to axions are those that provide an axial electric field component (transverse magnetic or TM modes). The expected power generated from axion-to-photon conversions in the cavity is given by [39]

$$\begin{aligned}
 P_a &= \left(\frac{\alpha_{\text{em}} c_a \gamma \gamma}{2\pi F_a} \right)^2 V B_0^2 \rho_a C_{lmn} \frac{1}{m_a} \min(Q_L, Q_a) \\
 &= 0.5 \times 10^{-26} \text{ W} \left(\frac{V}{500 \ell} \right) \left(\frac{B_0}{7 \text{ T}} \right)^2 C_{lmn} \left(\frac{c_a \gamma \gamma}{0.72} \right)^2 \\
 &\quad \cdot \left(\frac{\rho_a}{0.5 \times 10^{-24} \text{ g cm}^{-3}} \right) \left(\frac{m_a}{2\pi (\text{GHz})} \right) \min(Q_L, Q_a), \tag{9.13}
 \end{aligned}$$

where V is the cavity volume, B_0 is the magnetic field strength, ρ is the local axion mass density, m_a is the axion mass, C_{lmn} is a form factor which describes the overlap of the axial electric and magnetic fields of a particular TM_{lmn} mode, Q_L is the microwave cavities loaded quality factor (defined as center frequency over bandwidth) and Q_a is axion quality factor defined as the axion mass over the axion's kinetic energy spread. The mode-dependent cavity form factor is defined as

$$C_{lmn} = \frac{|\int_V d^3x \mathbf{E}_\omega \cdot \mathbf{B}_0|^2}{B_0^2 V \int_V d^3x \epsilon |\mathbf{E}_\omega|^2}, \tag{9.14}$$

where $\mathbf{E}_\omega(\vec{x})e^{i\omega t}$ is the oscillating electric field of the TM_{lmn} mode, $\mathbf{B}_0(\vec{x})$ is the static magnetic field and ϵ is the dielectric constant of the cavity space. For a cylindrical cavity with a homogeneous longitudinal $\mathbf{B}$ -field, the T_{010} mode yields the largest form factor with $C_{010} \approx 0.69$ [48].

The mass range of cosmological axions is currently constrained between a few μeV and meV scales which corresponds to converted photon frequencies between several hundred MHz and a hundred GHz. Initially, larger microwave cavities were designed to detect lighter axions. Recently, however, the search efforts move to few tens μeV up to 0.01 eV range. Here, however, the scan rate is problematic [3]. The scan rate is determined by the amount of time it takes for a possible axion signal to be detected over the microwave cavity's intrinsic noise and is governed by the Dicke radiometer equation [49],

$$\text{SNR} = \frac{P_a}{\bar{P}_N} \sqrt{Bt} = \frac{P_a}{k_B T_S} \sqrt{\frac{t}{B}}. \tag{9.15}$$

Here, P_a is the power generated by axion-photon conversions (Eq. (9.13)), $P_N = k_B B T_S$ is the cavity noise power, B is the signal bandwidth, t is the integration time, k_B is Boltzmann's constant and T_S is the system temperature (electronic plus

physical temperature). The scan rate for a given signal to noise is given by

$$\frac{df}{dt} = \frac{12 \text{ GHz}}{\text{yr}} \left(\frac{4}{\text{SNR}} \right)^2 \left(\frac{V}{5001} \right) \left(\frac{B_0}{7 T} \right)^4 C^2 \cdot \left(\frac{c_{a\gamma\gamma}}{0.72} \right)^4 \left(\frac{\rho_a}{0.45 \text{ GeV/cm}^3} \right)^2 \left(\frac{3K}{T_S} \right)^2 \left(\frac{f}{\text{GHz}} \right)^2 \frac{Q_L}{Q_a}. \quad (9.16)$$

One can see from Eq. (9.15) that even a tiny expected signal power can be made detectable by either increasing the signal power ($P_a \propto V B_0^2$), increasing the integration time t or minimizing the system noise temperature T_S . Technology and costs limit the size and strength of the external magnets and cavities and integration times are usually $t \sim 100$ seconds in order to scan an appreciable bandwidth in a reasonable amount of time. As a result, the majority of development has focused on lowering the intrinsic noise of the first stage cryogenic amplifiers.

Microwave receiver detectors

Initial experiments were undertaken by the Rochester–Brookhaven (RB) Collaboration [50] and by the University of Florida [51], but they were still factors of 10–100 times away from plausible axion model space. Since August, 2016, the second generation experiment Axion Dark Matter eXperiment (ADMX) at University of Washington is taking data. A more powerful third generation experiment CAPP (Center for Axions and Precision Physics, Institute of Basic Science) in Daejeon, Korea, is constructed now and will take data from sometime 2018. Both experiments utilize large/small microwave cavities immersed in a strong static magnetic field to resonantly convert axions to photons.

ADMX consists of an 8.5 Tesla superconducting magnet, 110 cm in length with a 60 cm clear bore. A 200-liter stainless steel microwave cavity plated in ultra-pure copper is suspended below a cryogenic stage in the center of the B-field. Power generated in the cavity is coupled to an adjustable antenna vertically input through the top cavity plate. Any signal is then boosted by extremely low noise cryogenic amplifiers before being sent through a double-heterodyne mixing stage. Here, the GHz range signal is mixed down to an intermediate 10.7 MHz, sent through a crystal bandpass filter, and then mixed down to audio frequencies at 35 kHz. This audio signal is then analyzed by fast-Fourier-transform (FFT) electronics which measure over a 50 kHz bandwidth centered at 35 kHz. There is also a “high resolution” channel in which the signal is mixed down to 5 kHz and sent through a 6-kHz wide bandpass filter. Time traces of the voltage output, consisting of 2^{20} data points, taken with a sampling frequency of 20 kHz is then taken, resulting in a 52.4 s sample with 0.019 Hz resolution [52].

Results from the initial run using HFET amplifiers have already probed plausible axion model space in the axion mass range between 2.3 and 3.4 μeV [48]. Results from a high resolution search have probed further into coupling space over a smaller

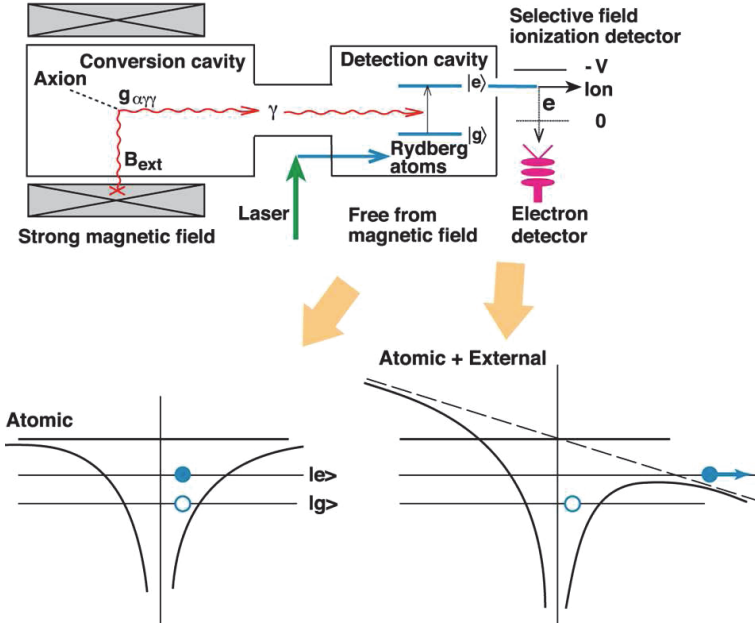


Fig. 9.12. General concept of the CARRACK experiment utilizing Rydberg atoms.

mass range, $1.98\text{--}2.17\ \mu\text{eV}$ [52]. As of this review, ADMX is scanning over the mass range corresponding to 800–900 MHz using SQUID amplifiers.

Pizza-cylinder cavity detector

Recently, a pizza-cylinder type multiple cavities is introduced to detect higher frequency region with the same magnet bore [116]. A cylinder enclosed in the magnet is evenly divided by metal partitions. This design is superior to the conventional multiple cavities within the cylinder: in terms of the detection volume, experimental set-up, and the phase-matching mechanism. Some analytic solutions and various simulation studies can be found in [116]. So this design seems promising for searching the high axion mass region up to $\sim 100\ \mu\text{eV}$ in the cavity-based experiments.

Rydberg atom detectors

The Cosmic Axion Research with Rydberg Atoms in Cavities at Kyoto (CARRACK) experiment has published proof of concept papers for their detection technique using Rydberg atoms [3, 53]. The experimental setup can be seen in Fig. 9.12. In it, rubidium atoms are excited into a Rydberg state ($|0\rangle \rightarrow |n\rangle$), and move through a detection cavity coupled to an axion conversion cavity. The spacing between energy levels is tuned, to the appropriate frequency utilizing the Stark effect and the Rydberg atoms large dipole transition moment ensures efficient photon

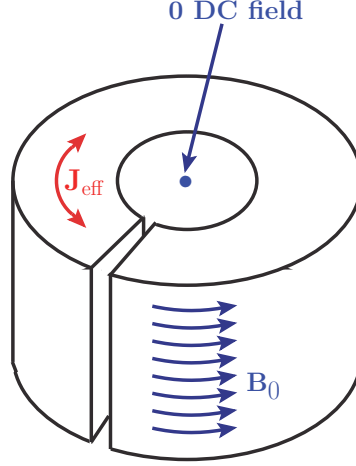


Fig. 9.13. A design of ABRACADABRA. At the center of cylinder the DC field vanishes, and an oscillating one due to the axion oscillation is to be detected.

detection (one photon per atom, $|ns\rangle \rightarrow |np\rangle$). The advantage of this system is that Rydberg atoms act as single photon detectors and thus do not suffer from quantum noise limitations. One disadvantage of this technique is that one cannot detect signals finer than the bandpass of the cavity, of order $\sim 10^{-5}$, which negates searches for late infall coherent axions.

Toroidal cavities

Toroidal cavities are also used for QCD axions at the axion window [54] and for the GUT axions with the proposal “A Broadband or Resonant Approach to Cosmic Axion Detection with an Amplifying B-field Ring Apparatus (ABRACADABRA)” [55]. For the QCD axion search, they try to detect the Primakoff effect in the cavity, as usual. For the GUT axions, one uses the unique toroidal geometry that at the center of the toroid the axion induced effective current,

$$\mathbf{J} = g_{a\gamma\gamma} \sqrt{2\rho_{\text{DM}}} \mathbf{B}_0 \cos m_a t, \quad (9.17)$$

is designed to be detected. The typical geometry for the GUT axion search is shown in Fig. 9.13.

aKWISP detector

The idea discussed below is in the primitive stage, and it can be modified significantly in the real detectors. Searches of weakly interacting slim particles (WISPs) have been proposed under the name of kinetic WISP (KWISP) detection [56], which was proposed to detect chameleons produced in Sun by exploiting their local density-dependent direct coupling to matter. Some ALPs models fit to this scheme for detection.

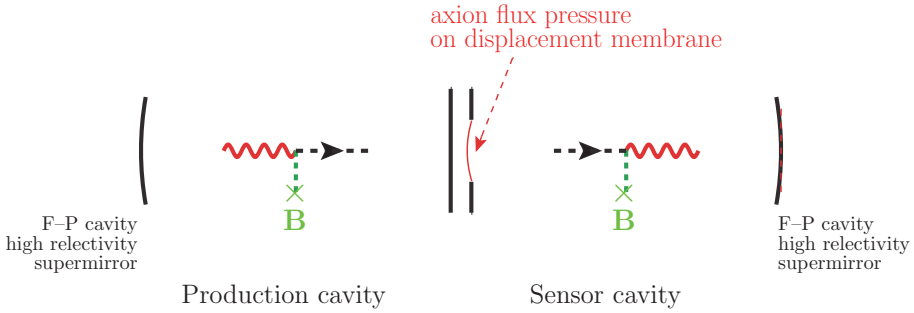


Fig. 9.14. A design of aKWISP.

The KWISP sensor consists of a thin and rigid dielectric membrane suspended inside a resonant optical Fabry–Perot (F–P) cavity. The advanced KWISP (aKWISP) is an axion production/sensor, consisting of two cavities, and two membranes are placed in the middle as shown in Fig. 9.14 [57]. The left membrane is the axion production membrane and the right membrane is the sensor membrane. The left membrane is oscillated with a mechanical frequency corresponding to the axion mass. At the resonant frequency of the force, corresponding to the axion mass, the laser beam produces axions via the Primakoff process. Produced axions travel freely, some to the right cavity. Axions in the right cavity produces electromagnetic waves corresponding to the axion mass, again by the Primakoff process.

The sensor (the right membrane) detects the frequency of the applied force. By monitoring the cavity characteristic (mechanical) frequencies, the tiny membrane displacements, caused by an applied force, are detected. The sensor transduces displacement (force) into an electrical signal with a gain proportional to the finesse of the F–P cavity. The prototype model of Ref. [56] uses a thin Si_3N_4 micromembrane placed inside an F–P optical cavity. But, it may be way short of detecting a QCD axion.

Finally, we point out that there is an ingenious method to probe the anthropic window of f_a , which uses an EDM search method in a storage ring [118]. The storage ring method uses a combination of $\mathbf{B}$ and tunable $\mathbf{E}$ fields to produce a resonance between the $g - 2$ precession frequency and the background axion field oscillation. The deuteron nucleus and proton beams can be used for this method.

9.4. Massive particles

9.4.1. Collider search of massive DM particles

If massive DM particles such as WIMPs are present, they can be tested by three processes as shown in Fig. 9.15 where χ and SM denote the WIMP and SM particles, respectively. Reading the diagram from bottom to top, it represents the production of WIMPs at particle accelerators. Reading the diagram from top to bottom, it

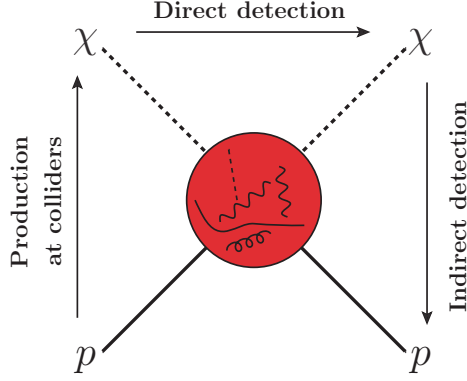


Fig. 9.15. Possible DM detection channels.

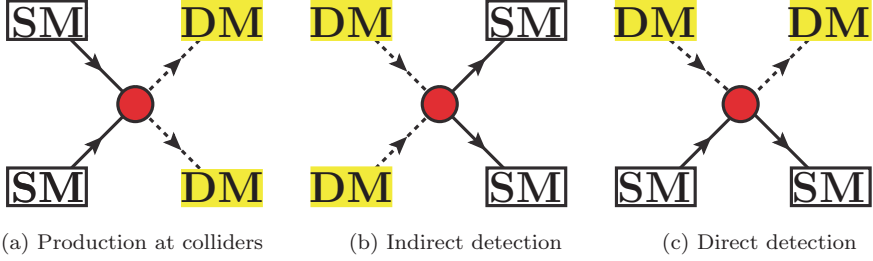


Fig. 9.16. WIMP detection: (a) collider production, (b) indirect detection, and (c) direct detection.

represents the signals from annihilation of WIMPs which will be discussed in Section 9.4.2. Reading the diagram from left to right, it represents the scattering of WIMPs to the SM particles the so-called *direct detection* of DM, which will be reviewed in Section 9.4.3.

Collider production of WIMPs is sketched in Fig. 9.16(a). Since 2008, the ATLAS and CMS experiments at Large Hadron Collider (LHC) at CERN have searched for WIMPs in proton–proton collisions. The LHC run-1 was operated at the center of energy of 7 TeV, and the LHC run-2 has so far operated at the center of energy of 8 TeV and 13 TeV. The WIMP search reactions are of the type

$$p + p \rightarrow \chi + \bar{\chi} + \cdots, \quad (9.18)$$

where $\bar{\chi} = \chi$ for a Majorana-type WIMP. In Eq. (9.18), $\cdots$ can be a hadronic jet (the so-called mono-jet), a photon or a leptonically decaying Z or W boson. The result so far obtained in the run-2 gives a WIMP mass lower bound at 400 GeV [59]. The 13 TeV run gives cross-section bounds for a relatively lightest SUSY particle

(LSP) [60],

$$\begin{aligned} \text{ATLAS: } 3.2 \text{ fb}^{-1}, \\ \text{CMS: } 2.3 \text{ fb}^{-1} \end{aligned} \tag{9.19}$$

in the pMSSM with 19 parameters. The 19-parameter pMSSM region is shown as light green in Fig. 9.18.

9.4.2. Indirect detection of WIMPs

In astrophysical objects such as stars, galaxies or Sun, DM particles can accumulate gravitationally in the long history of the Universe. In particular, at the galactic center (due to the huge DM density) and the galactic halo (due to scarce stars), the DM sources are looked for by means of indirect signals. Also, the nearby galaxy clusters or dwarf galaxies (called dwarf spheroidals) are possible objects to be looked for in favor of DM searches. This kind of secondary particle measurements is called “*indirect detection*” mechanism. Some examples for possible detection channels for annihilation and decay processes are

$$\begin{aligned} \chi + \bar{\chi} &\rightarrow \gamma + \gamma, \gamma + Z, \gamma + h, \text{ or} \\ \chi + \bar{\chi} &\rightarrow q + \bar{q}, W^+ + W^-, Z + Z, \end{aligned} \tag{9.20}$$

$$\begin{aligned} \chi &\rightarrow \gamma + \gamma, \gamma + Z, \gamma + h, \text{ or} \\ \chi &\rightarrow q + \bar{q}, W^+ + W^-, Z + Z. \end{aligned} \tag{9.21}$$

Some of the final products of (9.20) and (9.21) decay to e^+e^- , $p\bar{p}$, γ -rays, and neutrinos. Another mechanism to generate detectable charged particles, photons, and neutrinos from DM source is given by its decay. This indirect detection of astrophysical WIMPs is reviewed in [2].

The search of the indirect detection has been triggered by the PAMELA report on the rise of positron rate above 1.5 GeV up to 100 GeV [58] and by the AMS-II report [61]. But the tree-level estimate of the cross-section turns out to be about a factor of 10^{-2} – 10^{-4} times smaller than the observed excess at the PAMELA detector. One needs an enhancement if the favored LSP-type WIMP is the CDM source.

If the mother symmetry such as R -parity is exact, we consider only the annihilation process (9.20). Annihilations of two DM particles in the early Universe and now are determined by the same interaction, Fig. 9.16(b), but the kinematics are vastly different. The relative velocity of the two particles v_{rel} at the freeze-out temperature was about 0.3, but v_{rel} now is about 10^{-3} . So, the numerical values of the annihilation cross-sections may differ significantly. At the low velocity case, there is the so-called Sommerfeld enhancement [62]. For the case of Fig. 9.16(b), it was used first for the gluino LSP in Ref. [63], and later it was rechecked in [64]. In general, DM scenarios with many possibilities of force mediators, the enhancement

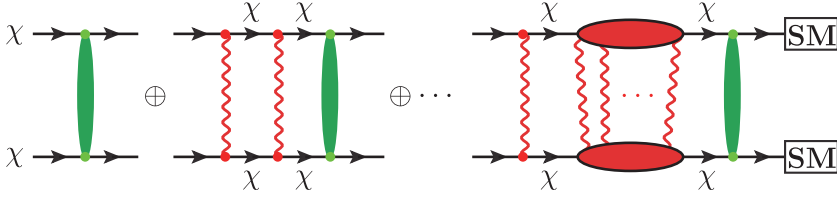


Fig. 9.17. Feynman diagrams for the Sommerfeld enhancement at low velocity. The green bullet shows Fig. 9.16(b) and the red bullets contribute to the enhancement.

at low velocities has been studied extensively after the PAMELA report [65]. The Sommerfeld enhancement factor is calculated from diagrams of the type shown in Fig. 9.17. The enhancement factor given from the red bullets is

$$S^0 = \frac{2\pi\alpha_X/v_{\text{rel}}}{1 - e^{-2\pi\alpha_X/v_{\text{rel}}}} \rightarrow \frac{2\pi\alpha_X}{v_{\text{rel}}}, \text{ in the limit of } \alpha_X \gg v_{\text{rel}}, \quad (9.22)$$

where α_X is the coupling strength of the force mediator and v_{rel} is the relative velocity of two annihilating DM particles. Note that it is not confirmed that the PAMELA rise is due to the indirect source of DM, but is likely due to the astrophysical sources such as nearby pulsars.

Detection of γ rays from the annihilation or decay of DM is a promising method for identifying the DM since photon direction is not changed during its propagation. Compared to the energy scale of the Fermi Gamma-ray Space Telescope (Fermi-LAT), detections of low energy gamma rays are proposed by AstroGAM [66], and detections of high energy gamma rays are proposed by the Cherenkov Telescope Array (CTA), the High Altitude Water Cherenkov Observatory (HAWC), the Large High Altitude Air Shower Observatory (LHAASO) [67], and the High Energy cosmic Radiation Detection facility (HERD).

9.4.3. Direct detection of WIMPs

Now, we discuss the direct detection of massive DM particles, which will be called detection of WIMPs even though some force mediators would not have the interaction strength comparable to G_F . This direct detection is one of the important keys to prove the WIMP nature on CDM.

The experimental situation on the direct detection of WIMPs has been reviewed excellently in Ref. [68]. In this chapter, we present only the key ideas on the direct detection which might be useful to those trying to get an idea on this issue.

For the LSP search, Fig. 9.18 shows succinctly the current experimental situation in the cross-section vs. mass plot together with the theoretical predictions in SUSY models [72, 73]. The region from the CMSSM calculation for the diagrams of Fig. 7.2 (b), is shown in the lower right corner of Fig. 9.18. Here, the unification point $M_{\text{GUT}} \simeq 2.5 \times 10^{16}$ GeV is used and for SUSY breaking parameters just universal gaugino mass $m_{1/2}$, the soft mass relation $m_0 = m_{\tilde{t}} = m_{\tilde{q}} = m_{H_u, d}$, and

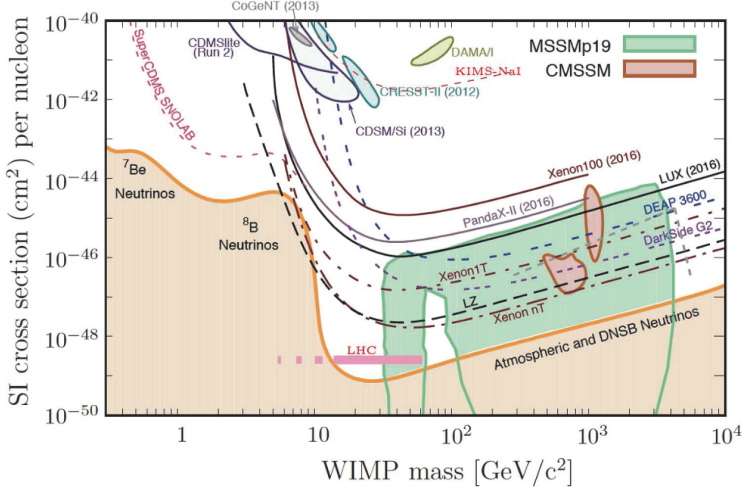


Fig. 9.18. Adapted from Ref. [69]. Updated bounds from direct DM searches sketched on neutrino backgrounds of Ref. [70]. The LHC bound, Eq. (9.19), and the prospect of the KIMS-NaI experiment [71] are shown in light red color. Also, the global analyses of SUSY predictions are given for the CMSSM [72] and the MSSMp19 [73].

the A -term are used. Note that some portion of the CMSSM and MSSMp19 regions are excluded by the LUX data [74, 75].

The differential recoil spectrum resulting from DM collision is [76]

$$\frac{dR}{dE_R}(E_R, t) = N_T \frac{\rho_{\text{DM}}}{m_\chi} \int d^3v v f(\mathbf{v}, t) \left(\frac{d\sigma}{dE_R} \right), \quad (9.23)$$

where N_T is the number of nucleons in the nucleus, m_χ is the WIMP mass, ρ_{DM} is the local DM density, $\mathbf{v}$ is the WIMP velocity in the Earth frame, and $d\sigma/dE_R$ is the WIMP–nucleus differential cross-section which is shown in the vertical axis of Fig 9.18. The nuclear recoil energy is $E_R = m_{\text{red}}^2 v^2 (1 - \cos \theta) / m_N$ where θ is the scattering angle, and m_N and m_{red} are the masses of the target nucleus and the WIMP (reduced mass), respectively. The E_R dependence or t dependence of dR/dE_R makes it possible to detect the E_R dependence or t dependence. Also, $f(\mathbf{v})$ makes it possible to look for the directionality, which is usually taken as the Boltzmann distribution

$$f(\mathbf{v}) = \frac{1}{\sqrt{2\pi}\sigma} e^{-|\mathbf{v}|^2/2\sigma^2}, \quad (9.24)$$

where the velocity dispersion of the WIMP is usually taken as $\sigma \approx 270 \text{ km s}^{-1}$. The integration region in Eq. (9.23) is usually taken from $v_{\text{min}} = \sqrt{m_N E_{\text{th}} / 2m_{\text{red}}^2}$ to v_{max} . v_{max} can be taken as the escape velocity in Earth [77], $v_{\text{esc}} \approx 544 \text{ km s}^{-1}$.

Now, we discuss three categories for the detection.

- Firstly, from Eq. (9.23) the approximate event rate as the E_R dependence is obtained [76],

$$\frac{dR}{dE_R}(E_R) = \left(\frac{dR}{dE_R} \right)_0 F^2(E_R) \exp\left(-\frac{E_R}{E_c}\right), \quad (9.25)$$

where $(dR/dE_R)_0$ is the event rate at zero momentum transfer, E_c is a characteristic energy scale which is determined by m_χ and the target mass, and $F^2(E_R)$ is the form factor correction. Equation (9.25) shows that the signal is dominated at the low recoil energy. Because of the form of Eq. (9.25), there are minima in the exclusion plots in Fig. 9.18.

- Second, the t dependence is commonly known as the *annual modulation*. Because Earth rotates around Sun, the speed of DM particles to Earth coming from the Milky Way is largest on June 2 and smallest in December. This velocity dependence on t can be measured as the DAMA group reported [37] which is shown in Fig. 9.18. The differential rate is [76],

$$\frac{dR}{dE_R}(E_R, t) \approx S_0(E_R) + S_m(E_R) \cos\left(\frac{2\pi(t - t_0)}{T}\right), \quad (9.26)$$

where t_0 can be taken as the 150th day of the year and T is the year period. Here, S_0 is the time-averaged rate and S_m is the modulation amplitude.

- Third, velocities of cosmic WIMPs to Earth are determined by three velocities: the circular velocity of halo DM v_c , the velocity of Sun around galactic center $v_\odot$ ($v_\odot \simeq \sqrt{2/3}v_c$), and Earth velocity around Sun v_E . The event rate is given by [78],

$$\frac{dR}{dE_R d\cos\gamma} \propto \exp\left(\frac{-[(v_E + v_\odot)\cos\gamma - v_{\min}^2]^2}{v_c^2}\right), \quad (9.27)$$

where γ is the angle defined by the direction of the nuclear recoil and the mean direction of the solar motion.

The second and third categories look for the relative magnitudes. On the other hand, the first category looks for the absolute magnitude, and most WIMP searches listed in Fig. 9.18 are in fact based on this first category. For the absolute magnitude, the reliable information on the nuclear form factors and the characteristic energy scale E_c are crucial.

Spins and form factors

The target nucleus is characterized by the nucleon numbers, the spin $\vec{S}$, the electromagnetic charge $Q \equiv eQ_{\text{em}}$, and the magnetic moment $\vec{\mu}$. In principle, the event

rate depends on all these quantities and the corresponding form factors. We will first discuss on the elastic cross-section and then show a caveat that the rate is lowered for the inelastic cross-section.

If the WIMP does not have magnetic moment, the rate then depends on the numbers of protons and neutrons and on the nuclear spin. For the spin-independent (SI) part, it is usually *assumed* for simplicity that protons and neutrons contribute equally to the scattering process. For a sufficiently low momentum transfer, these contribute in phase *coherently*, increasing the detection rate. For the spin-dependent (SD) part, only the unpaired nucleon spins contribute. Again, it is *assumed* that unpaired protons and neutrons contribute equally. If the Pauli exclusion principle is applied to protons and neutrons, only the odd number of protons or neutrons might be considered to this SD part. However, protons and neutrons are composite, and to apply the Pauli exclusion principle we must consider quarks with the color degrees of freedom. So, the detection rate is parameterized by

$$\frac{d\sigma}{dE_R} = \frac{m_A}{2\mu_A^2 v^2} (\sigma_0^{\text{SI}} F_{\text{SI}}^2(E_R) + \sigma_0^{\text{SD}} F_{\text{SD}}^2(E_R)), \quad (9.28)$$

where m_A and μ_A are the mass and reduced mass of the recoiling nucleus and σ_0 's are constants. The experiments so far performed, listed in Fig. 9.18, looked for the SI part. Noting that the form factors of protons and neutrons are different, the SI cross-section is split into the dependences on the proton (Z) and neutron ($A - Z$) numbers,

$$\sigma_0^{\text{SI}} = \sigma_p \frac{\mu_A^2}{\mu_p^2} [Z f^p + (A - Z) f^n]^2, \quad (9.29)$$

where $f^{p,n}$ are given by the WIMP-proton/neutron coupling. As commented above, usually $f^p = f^n$ is assumed. Because of the coherent effect mentioned above, $\sigma_0^{\text{SI}} \propto A^2$, and targets of heavy nucleus are effective in detecting WIMPs.

For the SD part, there are more parameters to be considered, and it is highly model dependent. The following simple expression for the SD part is usually used [68],

$$\sigma_0^{\text{SD}} = \frac{32}{\pi} \mu_A^2 G_F^2 [a_p \langle S^p \rangle + a_n \langle S^n \rangle]^2 \frac{J + 1}{J}, \quad (9.30)$$

where G_F is the Fermi coupling constant, J is the total spin of the nucleus, $a^{p,n}$ are the effective proton/neutron couplings with the WIMP, and $\langle S^{p,n} \rangle$ are the expectation values of spins of the proton/neutron groups, respectively. The above form (9.30) is a simplification, as one can see that there are 14 different operators in the effective field theory classification of WIMP-like interactions [79].

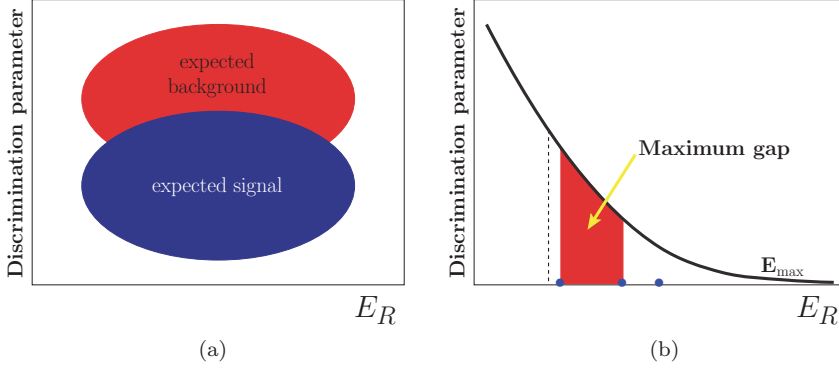


Fig. 9.19. WIMP direct detection illustration. The vertical axis is some ratio such as (number of phonons)/(number of photons) or (number of electrons)/(number of photons), etc., for an event.

Recoil energy dependence

Most experimental results are reported in the rate vs. the recoil energy plane, where the reduced mass of WIMP is calculated by

$$m_{\text{red}} = \sqrt{\frac{m_N E_R}{v^2 (1 - \cos \theta)}}. \quad (9.31)$$

If a candidate event in the scattering angle θ is found for the target nucleus mass m_N , the WIMP mass is calculated with Eq. (9.31). One may take $v \approx \sigma \simeq 270 \text{ km s}^{-1}$.

Generally, the backgrounds from electron recoils due to internal radioactivity or gamma-ray interaction from outside are high in the rate compared to the rate expected DM signal, the signals and backgrounds are not completely separated as shown in Fig. 9.19(a). When the accepted number of events are low, the absence of events in certain intervals (shown in Fig. 9.19(b)) is used to calculate the probability of not measuring DM events in that interval. For example, take the red maximum gap with a high probability of exclusion (2 events) and find one candidate event.

Observables and detection techniques

The elastic scattering of WIMPs off nucleus transfers energy to the target nucleus. This can be observed by three different signals: production of heat by the lattice vibration, excitations of the target atoms resulting in scintillation, and the direct ionization of target atom. It is also possible that some of these can be combined together in the same event.

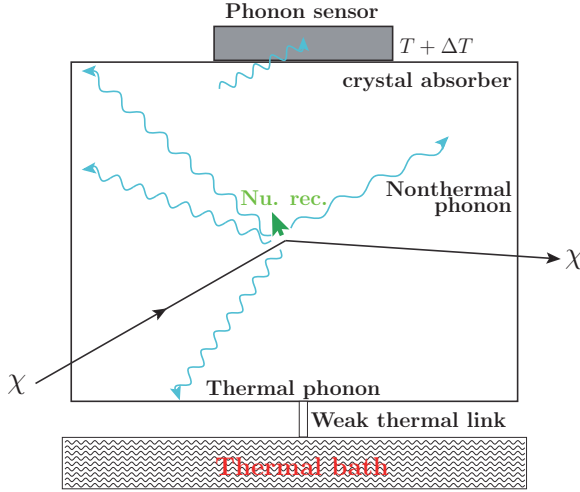


Fig. 9.20. A schematic view of cryogenic bolometer. The nuclear recoil energy shown as green arrow is gradually dissipated by creating nonthermal phonons.

Cryogenic bolometers

Cryogenic bolometers detect phonon signals created by the lattice vibration of crystals. The nuclear or electron recoil energy induced by a WIMP collision in the crystal is gradually dissipated, which causes a small increase of temperature: these detectors basically measure the temperature change ΔT at the sensor. A detection scheme is sketched in Fig. 9.20. Typical sensors are neutron transmutation doped (NTD), transition-edge sensor (TES), and metallic magnetic calorimeter (MMC).

In addition to the ΔT measurement, bolometric detectors measure another variables for particle discrimination.

The CDMS group used the Z -sensitive ionization and phonon-mediated (ZIP) detectors to measure ionization as well as phonon, using Ge, etc. [81, 82]. The CDMS II excluded 7 GeV WIMP with cross-section 10^{-41} cm^2 . Its later evolution to SuperCDMS, using an improved interleaved ZIP technology (iZIP), presented a stronger bound, for example the cross-section bound $1.2 \times 10^{-42} \text{ cm}^2$ for an 8 GeV WIMP [83]. Another detector of CDMS evolution is CDMSlite (CDMS low ionization threshold experiment), using only a single crystal of SuperCDMS, allowing a low energy threshold, whose bound is shown in Fig. 9.18 [84]. The EDELWEIS group [85] also measured ionization as well as phonon.

The CRESST-II experiment at LNGS, Italy [86], and AMoRE experiment in Yang Yang, Korea [88], also measure scintillation photons as well as phonons. The scintillation photons are measured by CaWO_4 TES crystals at CRESST-II. These experiments are devoted to a dedicated low mass region, for example a WIMP of 3 GeV with cross-section $0.8 \times 10^{-39} \text{ cm}^2$.

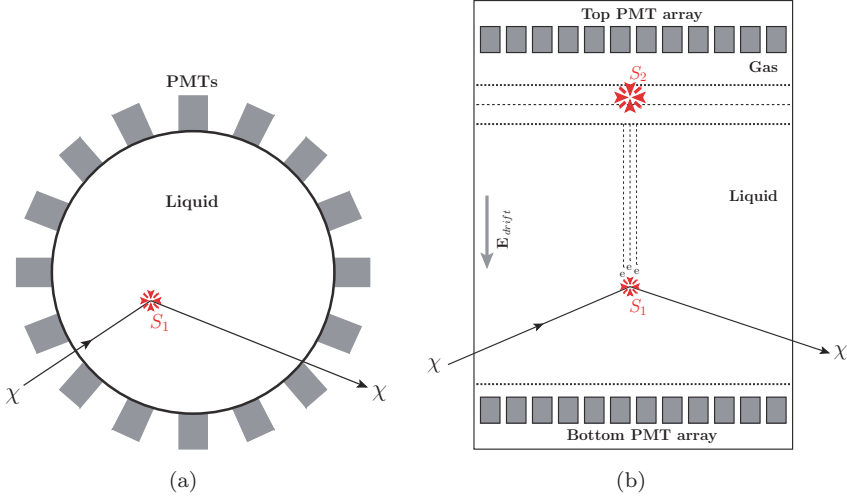


Fig. 9.21. Schematic views of noble gas detectors: (a) single phase and (b) two phase.

All these experiments measure two parameters: ΔT , and ionization or photon signal. The events measured in these experiments are presented in the discrimination parameters, such as the ratio of phonon and ionization(photon) signals, vs. recoil energy as sketched in Fig. 9.19.

Finally, we mention the bounds obtained by the CsI(Tl) crystal, which is notable in obtaining an SD cross-section bound with the cryogenic bolometer. CsI(Tl) is a commonly used scintillating crystal with ^{133}Cs and ^{127}I target elements that are sensitive to both SI and SD interactions. The KIMS experiment, performed at the Yangyang Underground Laboratory, Yang Yang, South Korea, obtained an SI cross-section limit of $3 \times 10^{-43} \text{ cm}^2$ at 70 GeV WIMP mass at 90% CL, and an SD cross-section limit of $2 \times 10^{-38} \text{ cm}^2$ at 80 GeV WIMP mass at 90% CL [89].

Detectors with liquid noble gases

DM detector technology based on liquid noble gases has matured to present the most stringent limits on WIMPs as shown in Fig. 9.18. The currently used noble gases for this purpose are liquid Xe (LXe) [90] and liquid Ar (LAr) [91].¹ The experimental setups are sketched in Fig. 9.21: (a) for the single-phase detectors and (b) for the two-phase detectors. One advantage of the single-phase method is to use an effective inner volume for self-shielding of backgrounds. However, there is a disadvantage that less information per event becomes available, in particular for the

¹Note that neon has been suggested as a medium for low-energy neutrino detection [92] and could potentially be employed in the search for WIMPs.

Table 9.1. Some properties of ^{54}Xe and ^{18}Ar .

	^{54}Xe	^{18}Ar
Mean atomic weight	131.3	40.0
Boiling point at 1 atm	165.0 K	87.3 K
Melting point at 1 atm	161.4 K	83.8 K
Liquid density	2.94 g cm^{-3}	1.40 g cm^{-3}
Dielectric constant of liquid	1.95	1.51
Volume fraction in Earth's atm	0.9×10^{-7}	0.934×10^{-2}
Radioactive isotopes	$^{54}\text{Xe}^{136}$	$^{18}\text{Ar}^{39}$
(half life)	$\tau_{1/2} = 2.16 \times 10^{21} \text{ yr}$	269 yr

case of LXe because there is no well-defined separation between electron and nuclear recoils based on the pulse shape of events. Information per event is obtained more easily in two-phase detectors which rely on the time-projection-chamber (TPC) technique [77]. Some of the nuclear and atomic properties of Xe and Ar are shown in Table 9.1 [77].

A collision of WIMP χ on a nucleus N excites the atom R surrounding N to an excited state R^* or to an ion R^+ . R , R^* , and R^+ instantaneously interact to produce a dimer R^{*2} . This dimer deexcites to settle down to the ground state by producing radiation in the ultraviolet regime,

$$R^{*2} \rightarrow 2 R + h\nu. \quad (9.32)$$

The scintillation $h\nu$, an ultraviolet single photon, from S_1 is detected at the photo-multiplier-tubes (PMTs) at the top and bottom PMT array in Fig. 9.21(b). In addition, in the two-phase method, S_2 located at the gas phase detects the electron signal gathered by the high field $\mathbf{E}_{\text{drift}}$ from the ionization process at S_1 located in the liquid phase of Fig. 9.21(b). The proportional scintillation photons at the top and bottom PMTs give the (x, y) information of S_1 . The z determination is obtained by the electron travel measured by the TPC. The (x, y, z) information obtained in this way enables one to reject the majority of backgrounds by the fiducial volume cuts.

The main backgrounds are caused by the environmental radioactivity including nuclear recoil from radon and its daughters in air, impurities in the detector, shield material, neutrons in (α, N) nuclear reaction and fission reaction, cosmic rays, and activation of detector materials by ionization from recoils of electrons trapped at surfaces during exposure at the Earth's surface. Fortunately, the detection techniques have matured enough now to give meaningful bounds [77].

The single-phase method is employed by the XMASS located at the Kamioka Observatory in Japan [93], and MiniCLEAN [94] and DEAP-3600 located at SNO-Lab, Sudbury in Canada [95]. The XMASS uses LXe and MiniCLEAN and DEAP-3600 use LAr. The two-phase method so far employed uses LXe: ZEPLIN [96], XENON100 [74], etc. The most strong limit is obtained by the Large Underground Xenon experiment (LUX) of the Stanford Underground Research Facility (SURF) in Lead, SD, USA, with the two-phase method at the $0.76 \times 10^{-45} \text{ cm}^2$ level [75].

The future projects aim at obtaining the SI cross-section at the level of 10^{-48} cm^2 . The XMASS collaboration plans 1 t (fiducial) single-phase detector, aiming at 10^{-46} cm^2 . The PandaX experiment with the two-phase method in China will use LXe with active mass of 2 t [100]. The XENON1T and XENONnT experiments with the two-phase method plan to reach down to the SI cross-section at the $2 \times 10^{-48} \text{ cm}^2$ level [97]. The next phase of LUX and ZEPLIN (LZ) program plans to have 7 t LXe detector with a goal reaching down to the $2 \times 10^{-48} \text{ cm}^2$ level after three years of data taking [98]. DARK matter WIMP search with Noble liquid (DARWIN) proposes to build one at the Laboratori Nazionali del Gran Sasso (LNGS), Italy, down to 10^{-49} cm^2 [99].

Detectors using superheated fluids: Bubble chambers

Bubble chambers used in some accelerator experiments in 1970s use the technology of using superheated liquids. Indeed, the first neutral current event at CERN was from the bubble chamber detector [101]. For the WIMP search, already there exist reports from this technology [102, 103]. Typical targets used are CF_3I , C_2ClF_5 , C_3ClF_8 , and C_4F_{10} all of which contain fluorine. Fluorine contains a large expectation value of proton spin content, which is sensitive to SD interactions to protons.

This technology uses a liquid in a superheated state, slightly below its boiling temperature, so that a small energy input creates an observable bubble. To create an observable bubble, however, a minimum energy deposit per unit volume is necessary. This requires an energy threshold for the bubble creation. An event is photographed with charge coupled device (CCD). The bubble chambers, operating just below its boiling temperature and with the character of explosive nature, are insensitive to the minimum ionizing backgrounds in the other direct detection experiments, by which most of backgrounds are rejected. For example, the COUPP experiment achieves $< 99.3\%$ efficiency using an acoustic sensor in rejecting the α backgrounds [104].

Because of the small sizes so far employed at the order of a few kg, the sensitivity reached by this method is not as sensitive as those SI cross-section limits obtained by liquid noble gases. But, these detectors using superheated fluids are effective in detecting the low mass WIMP particles.

The SIMPLE group with the energy threshold of 9 keV obtained SD cross-section limits of $0.57 \times 10^{-38} \text{ cm}^2$ at 35 GeV WIMP mass [103]. The PICO experiment (formed with PICASSO and COUPP experiments) operated at SNOLab obtained an SD cross-section limit of $0.9 \times 10^{-39} \text{ cm}^2$ at 40 GeV WIMP mass at 90% CL [105].

Annual modulation

The DAMA/LIBRA experiment, performed at the LNGS, has reported the annual modulation during 7 annual cycles, including the previous DAMA/NaI experiments,

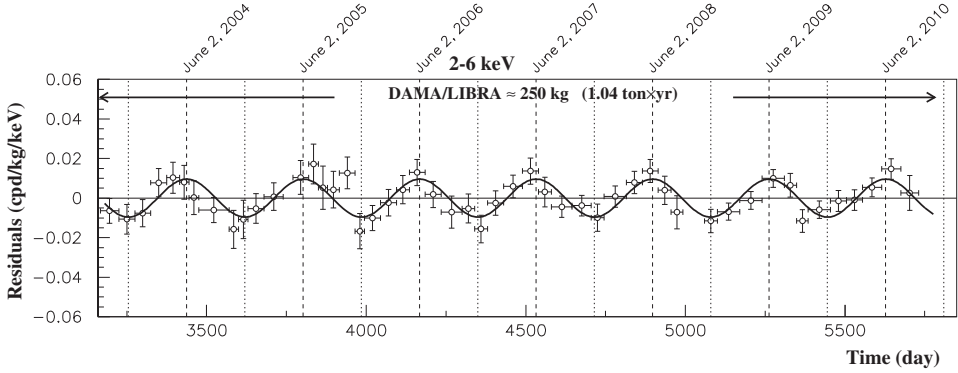


Fig. 9.22. The annual modulation reported by the DAMA/LIBRA group in the 2–6 keV energy interval as a function of the time [106]. The superimposed curve is the cosine function $A \cos \omega(t - t_0)$ with a period $T = 2\pi/\omega = 1$ year and $t_0 = 152.5$ day. The dashed vertical lines correspond to the maximum expected date, June 2, while the dotted vertical lines correspond to the minimum.

effectively for 14 annual cycles with 9.3σ CL [106]. The experiment used the highly radio-pure crystal NaI(Tl). The data for the 2–6 keV interval single hit events, which is preferred by the analysis [106], is shown in Fig. 9.22. The cross-section estimate is marked in Fig. 9.18. The Earth’s revolution around Sun marks the highest velocity (at which the modulation must be the largest) of WIMPs toward the detector on June 2 and the lowest velocity (at which the modulation must be the lowest) on December 2. The annual modulation parameters in (9.26) are determined as

$$T = 1 \text{ year}, \quad t_0 = 152.5 \text{ day}, \quad (9.33)$$

$$S_m(E_R) = 2 - 6 \text{ keV (within } 2\sigma \text{ contour)}, \quad (9.34)$$

which is presented in Fig. 9.22.

The high mass DAMA data is inconsistent with KIMS data [89]. On the other hand, the low mass DAMA data below 10 GeV at face value is consistent with the data of CoGeNT [107] and CRESST-II [108]. Note, however, that the backgrounds in the low mass region is difficult to remove completely. With the established CRESST-II technology, CRESST-III expects to reach $\sigma \sim 10^{-40} \text{ cm}^2$ for 1 GeV DM particles [109]. Another experiment using an NaI(Tl) crystal should be performed to check the DAMA signal.

Summary of WIMP detection experiments

In Fig. 9.23, the direct detection experiments are summarized with nuclear targets and three probing methods (shown in yellow boxes) and the collaboration groups employing the methods [110]. Pro/cons of these methods are written just above/below the yellow boxes.

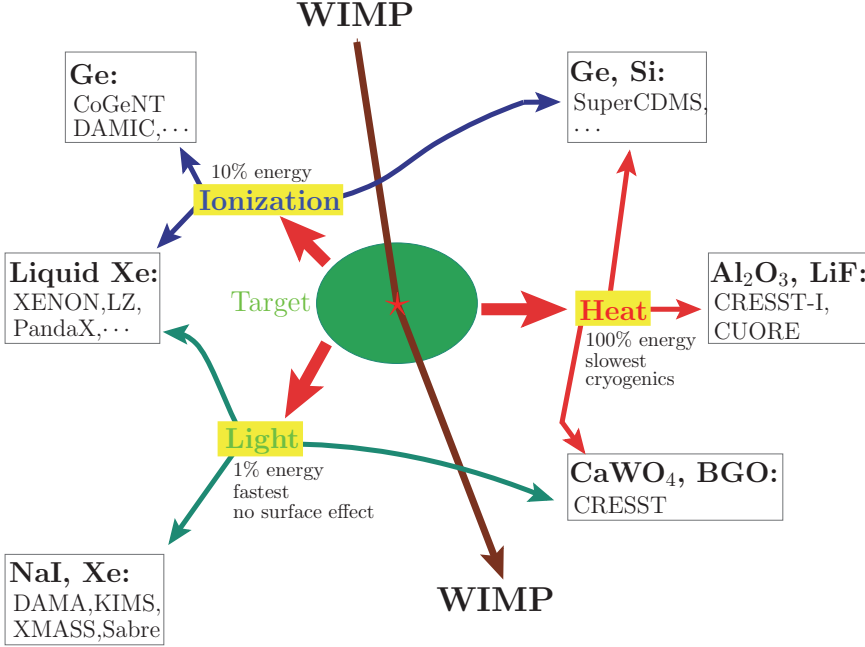


Fig. 9.23. A summary of WIMP direct detection experiments [110].

Magnetic moment of WIMP

So far we considered the contact interaction. But q^2 -dependent interactions may be applicable to DM. The most popular WIMP is the LSP which is supposed to be a Majorana particle. However, we cannot rule out a possibility of Dirac fermionic DM in which case an appreciable magnetic moment of the DM particle can be present. In fact, the magnetic moments of neutral fermions were considered for a long time since the time of weak neutral currents [111] up to the present age of DM [112].

One notable feature in the scattering through magnetic moment of neutral fermion is that it has a larger cross-section for a lower momentum photon exchange. In this regard, we note that direct detection experiments of DM can constrain the DM magnetic dipole moment. The CDMS II experiment [113] can be used for this. The SI cross-section is obtained as [114]

$$\frac{d\sigma}{dE_{\text{rec}}} = \frac{2M}{\pi v^2} (Zf_p + (A - Z)f_n)^2 F^2(E_{\text{rec}}), \quad (9.35)$$

where $f_p \simeq f_n \simeq 10^{-8} \text{ GeV}^{-2}$ are the SI couplings of WIMPs to protons and neutrons, respectively, the SI form factor $F(E_{\text{rec}}) = 3e^{-\kappa^2 s^2/2} (\sin(\kappa r) - \kappa r \cos(\kappa r)) / (\kappa r)^3$, with $s = 1 \text{ fm}$, $r = \sqrt{R^2 - 5s^2}$, $R = 1.2A^{1/3} \text{ fm}$, and $\kappa = \sqrt{2m_n E_{\text{rec}}}$. In Fig. 9.24, using several nucleus magnetic moments of Table 9.2, the magnetic moment hypothesis is compared to the CDMS II data. We observe that

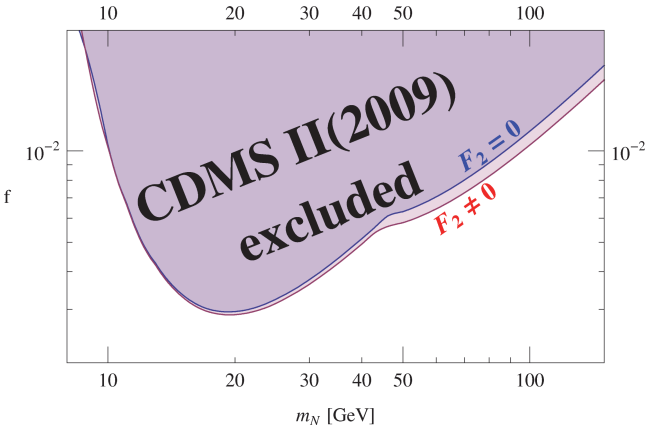


Fig. 9.24. Figure taken from [114] for the allowed region of the DM magnetic moment f vs. the DM mass m_N . f is the magnetic moment of N in units of the N Bohr magneton, $e/2m_N$. The upper colored regions are excluded for $F_2 = 0$ and $F_2 \neq 0$, respectively, with the 90% CI for the CDMS II data [113]. Note that there was a typo in Eq. (9) of [114], missing x inside the integral.

Table 9.2. Magnetic moments μ of several target nuclei used in cryogenic detectors. Here, $\mu_N = e/2m_p$. The nuclear spin is denoted as superscripts. F_2 is the half of the conventional definition, $F_2 = \frac{1}{2}F_2^{\text{st}}$.

	$\text{O}(8,16)^3$	$\text{Na}(11,23)^{\frac{3}{2}}$	$\text{Si}(14,28)^2$	$\text{Ge}(32,73)^{\frac{9}{2}}$
μ/μ_N	1.66812	2.21752	1.1218	-0.879467
F_2	4.83	13.36	4.02	-36.32
	$\text{I}(53,127)^{\frac{5}{2}}$	$\text{Xe}(54,131)^{\frac{3}{2}}$	$\text{Cs}(55,133)^{\frac{7}{2}}$	$\text{W}(74,183)^{\frac{1}{2}}$
μ/μ_N	2.81327	0.692	2.58	0.117785
F_2	94.56	6.52	83.93	-26.30

the hypothesis does not give a significant deviation from the case of zero magnetic moment.

Another study shows that the DM magnetic moment is ruled out independently of dark halo properties [115]. So, at the present level of experimental accuracy, we can neglect the effects of DM magnetic moment.

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